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# Evaluation of the PEM-2 (Pollution Episodic Model Version 2) Using the 1982 Philadelphia Aerosol Field Study Data Base

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# EVALUATION OF THE PEM-2 USING THE 1982 PHILADELPHIA AEROSOL FIELD STUDY DATA BASE

by

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16. ABSTRACT

This report describes an evaluation of the Pollution Episodic Model Version 2 (PEM-2) using measurements obtained from 29 days of the Philadelphia Aerosol Field Study. The model performance was determined by comparing predicted 12-h and 24-h average concentrations against corresponding obverved values at six monitoring sites for four pollutant species; particulate total mass, fine sulfate and $SO_2$ . A first-order chemical transformation of $SO_2$ to sulfate was considered, in addition to the direct emission, dry deposition, and settling of the pollutant species. The model domain covered 80km X 80km with 32 X 32 grid cells which included 300 major point sources and 289 area sources for the Philadelphia urban area. Hourly meteorological observations and hourly emissions were input to the model.

Statistical measures of difference and correlation paired in time and space revealed that the particulate species were simulated closely. These results, however, must be interpreted with caution since the background concentrations exceeded the local urban source contributions. Tables of statisical and regression analyses results as well as graphical displays of predicted and observed concentrations are presented and discussed.

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## ABSTRACT

The Pollution Episodic Model Version 2 (PEM-2) is an urban-scale model capable of predicting short term ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants at multiple receptors. The two pollutants may be chemically coupled through a first-order chemical transformation. PEM-2 is intended for urban particulate modeling, and for studies of the atmospheric transport, transformation, and deposition of pollutants to assess the impact of existing or new sources or source modifications on air quality.

This report describes an evaluation of the PEM-2 using Philadelphia Aerosol Field Study (PAFS) data for 29 days in the summer of 1982. The model's performance is judged by comparing the calculated 12-hour and 24-hour average concentrations with the corresponding observed values for four pollutant species, namely, $SO_2$, sulfate, fine and coarse total mass. The calculated and observed diurnal variations of hourly $SO_2$ concentrations at each of the six PAFS stations are also compared. A first-order chemical transformation of $SO_2$ to sulfate is considered in the calculations in addition to the direct emission and dry deposition of all four pollutant species. The model domain, covering 80 km x 80 km with 32 x 32 grid cells, includes 300 point sources and 289 area sources in the Philadelphia urban area. Hourly meteorological and emission data are used as inputs to the model.

Statistical tests for evaluation of model performance include standard measures of differences and correlation between observations and calculations paired in space and time. For each pollutant, scatterplots of calculated 12-hour average concentrations and differences versus observed concentrations are presented; a linear regression line is determined and evaluation statistics are tabulated. Additional plots and tables, examining the model performance for daytime, nighttime, and daily mean concentrations (averaged over all PAFS stations) are given. The diurnal variations of $SO_2$ concentrations (averaged over the evaluation days) are also compared at each station.

The emphasis in this evaluation is on particulate species for which the model performs well; the variations of 12 and 24-hour mean particulate concentrations over the evaluation period are simulated closely. These results, however, should be interpreted with caution since the background concentrations far exceed the urban source contributions to the particulate concentrations in Philadelphia. The model performance for $SO_2$ is better during daytime than at nighttime, and generally better at the suburban stations than at downtown stations which are impacted heavily by the urban area sources.



The work described in this report was performed by NOAA's Atmospheric Turbulence and Diffusion Division in partial fulfillment of an Interagency Agreement with the U.S. Environmental Protection Agency. This work, covering the period January 1984 to June 1985, was completed as of June 30, 1985.

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# SECTION 1

# INTRODUCTION

The U. S. Environmental Protection Agency (EPA) recently proposed revisions to the National Ambient Air Quality Standard (NAAQS) for inhalable particulate (IP) matter which would base the primary, health-related standard on particles smaller than 10 microns aerodynamic diameter (PM-10). As part of the effort to control urban particulate emissions, EPA sponsored the development and evaluation of an improved urban scale model capable of simulating the transport, diffusion, and deposition of particulate matter.

The Pollution Episodic Model Version 2 (PEM-2) described by Rao (1985) is an urban scale (10-50 km) model capable of predicting short term (1-24 hr) ground-level concentrations (GLC) and deposition fluxes of one or two gaseous or particulate reactive pollutants in an urban environment with multiple point and area sources. It is intended primarily for particulate modeling, and also for studies of the atmospheric transport, transformation, and deposition of acidic, toxic, and other pollutants to assess the impact of existing or new sources or source modifications on urban air quality. The PEM-2 concentration algorithms (Rao, 1983) explicitly account for the effects of dry deposition, sedimentation, and a first-order chemical transformation.

PEM-2 is based on the Pollution Episodic Model (PEM) developed by Rao and Stevens (1983). The latter, in turn, is based on the Texas Episodic

Model Version 8 (TEM-8) developed by the Texas Air Control Board (1979) for the atmospheric dispersion of non-reactive pollutants over a perfectly reflecting (non-depositing) surface. Rao (1985) discussed the key differences between these various models, and gave the algorithms, computational techniques, capabilities, limitations, and input/ouput parameters of PEM-2. Pendergrass and Rao (1984) described an evaluation of PEM using the St. Louis Regional Air Pollution Study (RAPS) data.

This report describes an evaluation of PEM-2 using the data from EPA's 1982 Philadelphia Aerosol Field Study (PAFS). This evaluation is designed to test the performance of the model by comparing its concentration estimates to the measured air quality data, using appropriate statistical measures of performance.

Twenty nine days (from July 16 to August 13, 1982) in the Philadelphia data base are utilized for the PEM-2 evaluation. The model performance is judged by comparing the calculated average concentrations with the corresponding observed values for the following pollutant species:

1. $SO_2$
2. Sulfate particles
3. Fine total mass
4. Coarse total mass

The cut-point size between fine particle (FP) and coarse particle (CP) total mass fractions is 2.5 microns. A first-order chemical transformation of $SO_2$ to fine sulfate is considered in the calculations in addition to the direct emission and dry deposition of all four pollutant species. For each pollutant, several plots examining the model performance are given, and the model evaluation statistics are tabulated.

## SECTION 2

## PHILADELPHIA DATA BASE

The 1982 Philadelphia Aerosol Field Study has been sponsored by the EPA to obtain detailed data bases on emissions and surface air concentrations of gases and particles, and concurrent meteorological conditions, with adequate temporal and spatial resolution to evaluate source and receptor models, including PEM-2, which are capable of predicting short term concentrations of particles. The emissions of primary particulate matter, and pollutants that undergo chemical transformation in the atmosphere to form secondary particulates are of special interest. Therefore, the study was designed to obtain data on total particulate mass, sulfate, and $SO_2$. Philadelphia was chosen for this study because it has a good mix of industrial emissions, and it was the site of an earlier program for evaluation of EPA's Urban Airshed photochemical oxidant model.

The PAFS experiment was conducted from July 14 to August 14, 1982. From this data base, detailed emission inventories, and meteorology and concentration measurements for twenty nine days are supplied by the EPA for PEM-2 evaluation. The evaluation days are listed in Table 1. The PAFS experiment and data base have been described in detail in other publications referred to below, and will not be discussed here; only the data used in the evaluation of PEM-2 and other relevant information will be described in this section.

TABLE 1

PEM-2 Evaluation Days of PAFS Data.

| Day | Date | Julian Day |
|---|---|---|
| 1 | July 16, 1982 | 197 |
| 2 | 17 | 198 |
| 3 | 18 | 199 |
| 4 | 19 | 200 |
| 5 | 20 | 201 |
| 6 | 21 | 202 |
| 7 | 22 | 203 |
| 8 | 23 | 204 |
| 9 | 24 | 205 |
| 10 | 25 | 206 |
| 11 | 26 | 207 |
| 12 | 27 | 208 |
| 13 | 28 | 209 |
| 14 | 29 | 210 |
| 15 | 30 | 211 |
| 16 | 31 | 212 |
| 17 | August 1, 1982 | 213 |
| 18 | 2 | 214 |
| 19 | 3 | 215 |
| 20 | 4 | 216 |
| 21 | 5 | 217 |
| 22 | 6 | 218 |
| 23 | 7 | 219 |
| 24 | 8 | 220 |
| 25 | 9 | 221 |
| 26 | 10 | 222 |
| 27 | 11 | 223 |
| 28 | 12 | 224 |
| 29 | 13 | 225 |

## EMISSIONS

Hourly emission inventories for point and area sources in the Metropolitan Philadelphia area during the PAFS monitoring period are developed by Engineering-Science (ES) of Fairfax, Virginia. The inventories are listed for FP total mass (diameter < 2.5 microns), CP total mass (2.5 - 10 microns), primary sulfate particles, and sulfur dioxide. The primary sulfate data are found from a variety of industrial processes, and its emission factors are expressed as multipliers of $SO_2$ values on a weight basis or as percent of flyash. These data are for total sulfates which include the sulfuric acid aerosol. No data are found on sulfate particle sizes. Because these are thought to be in the lower end of the IP size range, ES (1984) assumed that all sulfate particles are less than 2.5 microns in diameter. Therefore, emission data on coarse primary sulfate particles are not available, and coarse sulfate emissions are assumed to be zero in this evaluation.

The emission inventories are supplied on two magnetic tapes, the first with 300 major point sources, and the second with 289 area sources; the latter are given on a square grid with 17 x 17 cells each of which is a square of side 2.5 km. This emission grid covers the Philadelphia county and portions of Bucks, Chester, Delaware, and Montgomery Counties in Pennsylvania, and Burlington, Camden, and Gloucester Counties in New Jersey. Though this area is smaller than the Air Quality Control Region (AQCR), the grid encompasses the Philadelphia urban area including all of Philadelphia County to the North and East, and extends well beyond the monitoring site locations to the West and South, thus retaining all the emission data important for model evaluation.

In addition, ES provided emission data for minor point sources and fugitive particulate matter on a third tape, and for mobile sources on a fourth tape. These emission data are given on a square grid with 17 x 17 cells each of which is a square of 2.5 km side. This grid coincides with the area source grid, so that these emissions can be easily merged with area sources in the model calculations. Highway vehicle emissions data are generated by the Delaware Valley Regional Planning Commission (DVRPC) under subcontract to ES. The latter conducted limited source testing and collected silt loading samples from selected paved roads to provide site-specific data in Philadelphia for model evaluation.

The point source emission data contained the stack identification, its location in UTM (x,y) coordinates, stack parameters such as height, diameter, plume-exit velocity and temperature, and emission rates of the four pollutants (SO2, sulfate, fine mass, and coarse mass) in g/s. The area source emission data included the county code, grid cell number, location of southwest corner of the source in UTM (x,y) coordinates, and emission rates (in g/s) of the four species from each grid cell.

The major point sources in Philadelphia are electric utilities using oil and coal-fired boilers , municipal incinerators, oil refineries, metal and chemical industries, grain elevators, etc. The stack heights are generally below 100 m. Outside a 42.5 km x 42.5 km inventory area, ES selected only about 50 (out of 300) major point sources with $SO_x$ or total mass emissions above a cutoff value of 500 tons per year. All other point sources with relatively lower emissions or farther away from the monitoring sites are classified as minor point sources. The area sources consist of residential, commercial, industrial, and agricultural emissions, and

releases from transportation, incineration, construction, and other activities. ES developed procedures to generate hourly emission rates using data they collected within the framework of the PAFS study. For a discussion of these procedures and additional details of the point and area source inventories, the emissions report by Engineering-Science (1984) should be consulted.

It should be noted that these emission data do not represent real time conditions. For example, the precipitation events are not taken into account in developing the hourly emission estimates. The use of relatively large (2.5 km square) grid cells in the study complicates model evaluation since impacts from paved roads very near the monitors are likely to be the most significant contributions. Model results should be interpreted keeping these limitations in mind.

## CONCENTRATIONS

The ambient air monitoring network in the PAFS study was operated by PEDCO Environmental, Inc. of Cincinnati, Ohio. The actual period of data gathering lasted from 6 a.m. Eastern Daylight Time (EDT), July 14 to 6 a.m., August 14, 1982. The locations and characteristics of the six monitoring sites shown in Fig. 1 are described below:

Site 5

Philadelphia, PA
Community Health Services Building
500 South Broad Street
Center City - Commercial

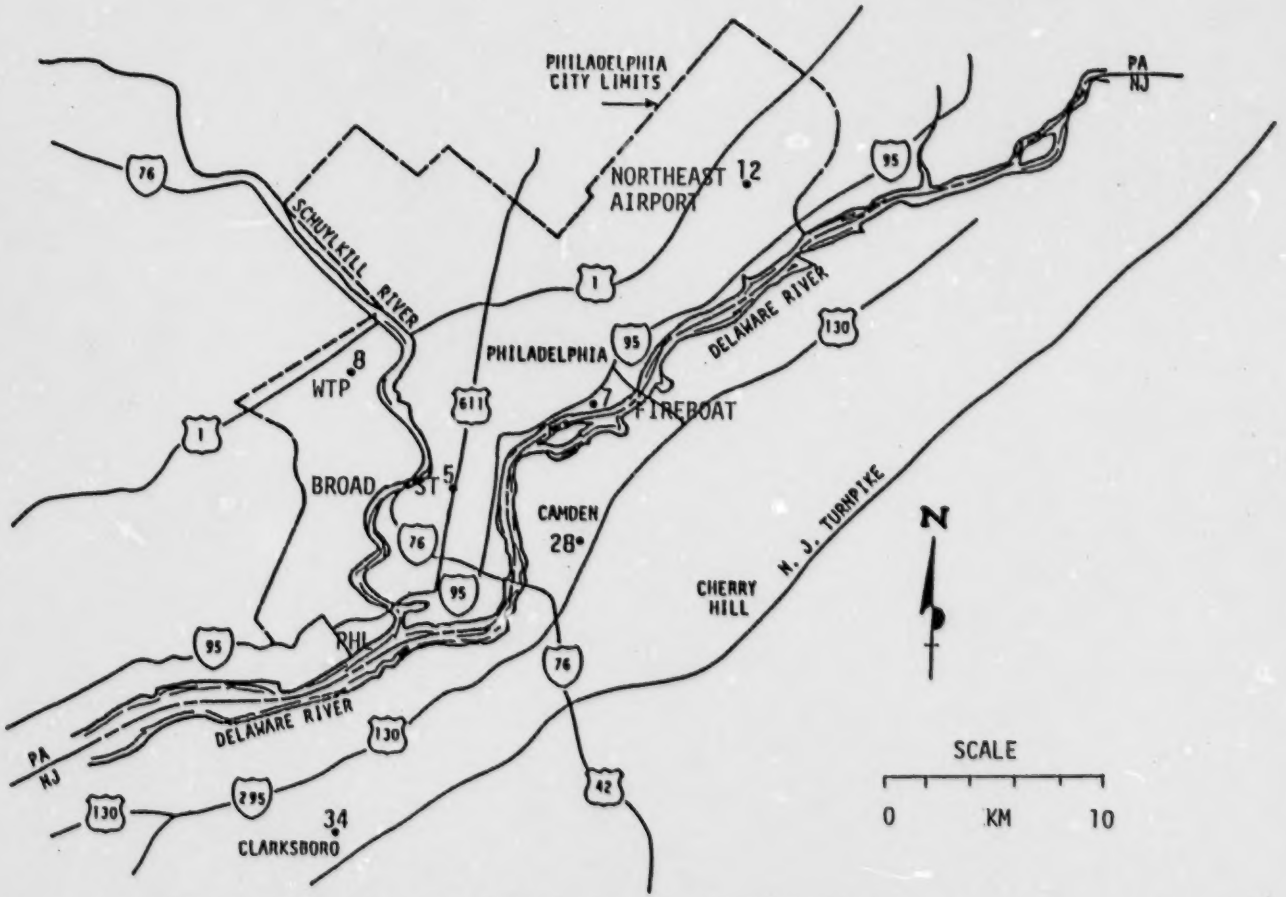


Figure 1. Philadelphia area map with locations of monitoring stations in PAFS field program. Location of the Philadelphia International Airport (and the National Weather Service station) is denoted by PHL.

Site 7

Philadelphia, PA
Fire Boat Station
Alleghany Ave. & Delaware River
Suburban - Industrial

Site 8

Philadelphia, PA
Water Treatment Plant
Ford Road & Belmont Ave.
Suburban - Residential

Site 12

Philadelphia, PA
Philadelphia Northeast Airport
Grant and Ashton Road
Suburban - Rural

Site 28

Camden, NJ
Institute for Medical Research
Copewood and Davis Streets
Suburban - Residential

Site 34

Clarksboro, NJ
Shady Lane Home
Cohawkin Road and County House Road
Suburban - Rural

The monitors at Site 5 are located on top of a building (11 m above street level) and are shielded to the south by a 2.5 m high building extension. Therefore, these monitors probably are not collecting representative samples from either the street-level or the building-top level. Site 7 is the most impacted by fugitive dust due to nearby truck terminals and heavy traffic on an adjacent paved road. The exact location of the roadway and construction-related emissions are not input to the model. Site 8 is affected by particulate emissions from a county maintenance yard with unpaved roads and aggregate storage piles. Site 12,

located near an area used for plane parking, is affected by heavy traffic on roads in the vicinity as well as airport operations and nearby small point sources. Site 28 is expected to be significantly impacted by paved road emissions, and Site 34 by a number of large point sources in the vicinity.

The measurements at the six sites listed above consist of the following:

1. Continuous gas monitoring of sulfur dioxide ($SO_2$), nitric oxide (NO), nitrogen dioxide ($NO_2$), non-methane organic carbon (NMOC), ozone ($O_3$), and carbon monoxide (CO), to obtain 1-hour average concentrations.
2. Particulate mass sampling twice daily at each site to obtain two 12-hour average concentrations, one for daytime (6 a.m. to 6 p.m.) and the other for nighttime (6 p.m. to 6 a.m.).
3. Meteorological data - wind speed, wind direction, doppler sodar data (at Site 28 until August 5, then relocated at Site 8), and minisondes (at Site 28 only).

These measurements are designed to obtain sufficient data to model FP and CP total mass, and sulfate concentrations on a 12- and 24-hour basis. $SO_2$ is monitored hourly to determine the chemical transformation contribution to the sulfate concentration. The other gases, namely, NO, $NO_2$, NMOC, and $O_3$ are monitored to establish sulfate mass formation via photochemical mechanisms. The study is conducted 24 hours a day to obtain data for modeling diurnal variations in sulfate formation. Sites 28 and 34 are operated by the State of New Jersey, and the other four sites by the City of Philadelphia. PEDCO installed and operated additional monitoring equipment for PAFS to supplement the instrumentation available at each site.

The continuous gas analyzers for $SO_2$ are either Beckman 953 or TECO Series 43; the particulate monitors are EPA's high-volume or dichotomous filter samplers. For the duration of PAFS, PEDCO operated the various monitors, recorders, and data acquisition systems, and performed the necessary checks, audits, and calibrations called for in the Quality Assurance (QA) Project Plan for the field study. For details on these procedures and instrumentation used in PAFS, the reader is referred to the report by PEDCO (1983).

For PEM-2 evaluation, the measured concentrations of $SO_2$, fine and coarse sulfate particles, and FP and CP total mass from the six monitoring sites of PAFS are provided by EPA on a magnetic tape. All concentrations, except $SO_2$, are 12-hour averages; $SO_2$ data are 1-hour averages.

## METEOROLOGY

Each of the monitoring stations is equipped with continuous wind speed and direction instruments. Data from each instrument are collected on strip chart recorders and data acquisition system. Aerovironment, Inc. (AV) performed thrice daily (4 a.m., 10 a.m., 4 p.m.) soundings of pressure (height), temperature, and wet-bulb depression (relative humidity) at Site 28 using an airsonde system developed by the Atmospheric Instrumentation Research (A.I.R.). Upper air wind data are obtained by using a theodolite to track the balloon that lifts the airsonde. To monitor upper air meteorology, a monostatic Doppler acoustic sounder is operated by AV to provide 15 minute averages of horizontal wind speed and direction at 30 m height increments up to 1 km.

The wind speed and wind direction data recording systems malfunctioned during the PAFS experiment; the surface meteorological measurements at the six sites are either missing or appear to be of dubious quality. Therefore, EPA has decided to use the hourly surface winds and temperatures observed at the Philadelphia International Airport (PHL) National Weather Service (NWS) Station (see Fig. 1) as input data for PEM-2 evaluation. A magnetic tape of these data consisting of hourly values of wind speed and direction, temperature, stability class, and mixing heights has been provided by the EPA. For each hour, the Pasquill-Gifford (PG) stability class and the two sets of mixing heights are determined by the RAM preprocessor (RAMMET), following a procedure described by Turner and Novak (1978). Morning and afternoon mixing heights required by RAMMET are derived from the observed airsonde temperature profiles as the base of the elevated inversion.

The values of the potential-temperature gradient above the mixing height are also determined from the temperature profiles for use in the optional new plume-penetration schemes of PEM-2 (see, Rao, 1985). The meteorological data are compiled into data files suitable for input to PEM-2; for example, stability class 7 (PG class G) in the RAMMET output is reset as stability class 6 (PG class F) in PEM-2.

Figure 2 shows the daytime wind distribution from the NWS data at PHL during the PAFS experiment. The surface winds during the day are predominantly from the southwest (WSW to SSW), with speeds ranging mostly from 2 to 6 m/s. The nighttime (6 p.m. to 6 a.m.) wind rose presented in Fig. 3 also shows a dominant southwesterly component. The major point sources in the Philadelphia area are distributed along a line oriented

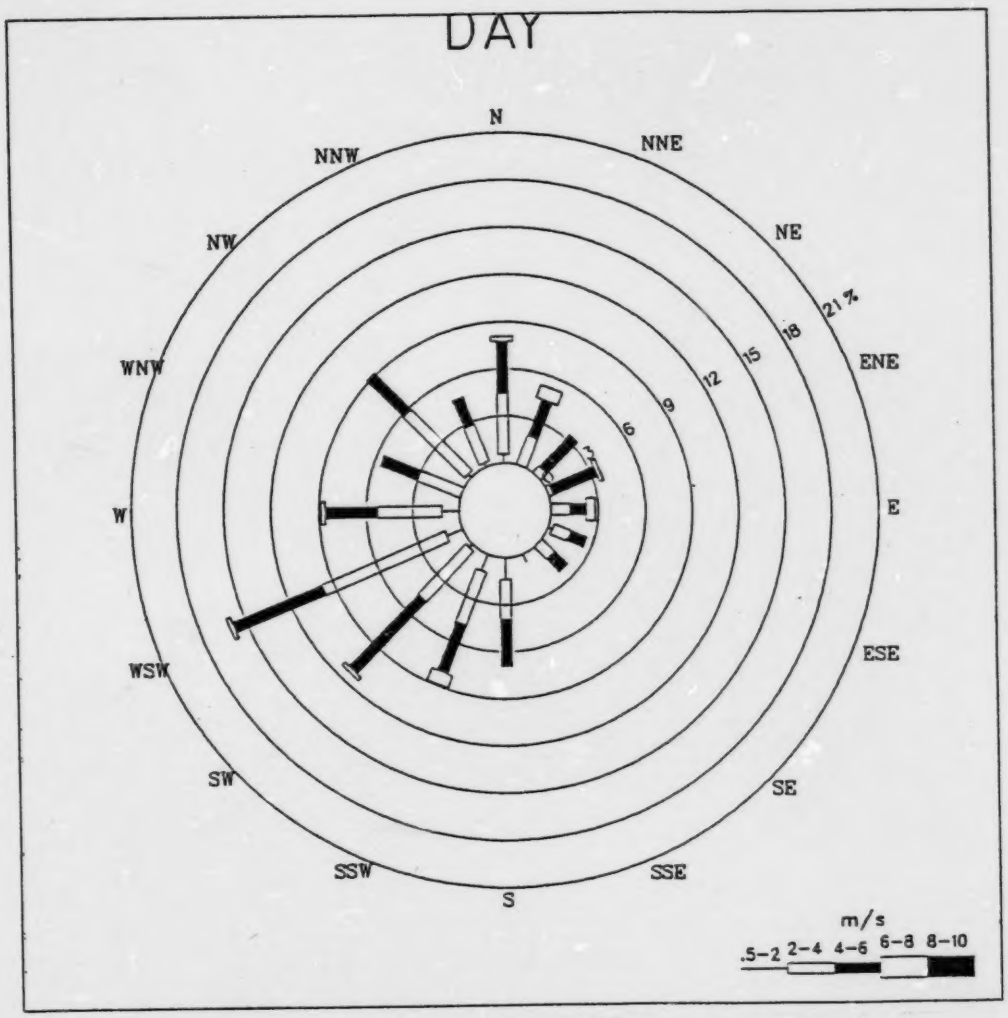


Figure 2. Average daytime wind distribution during PAFS.

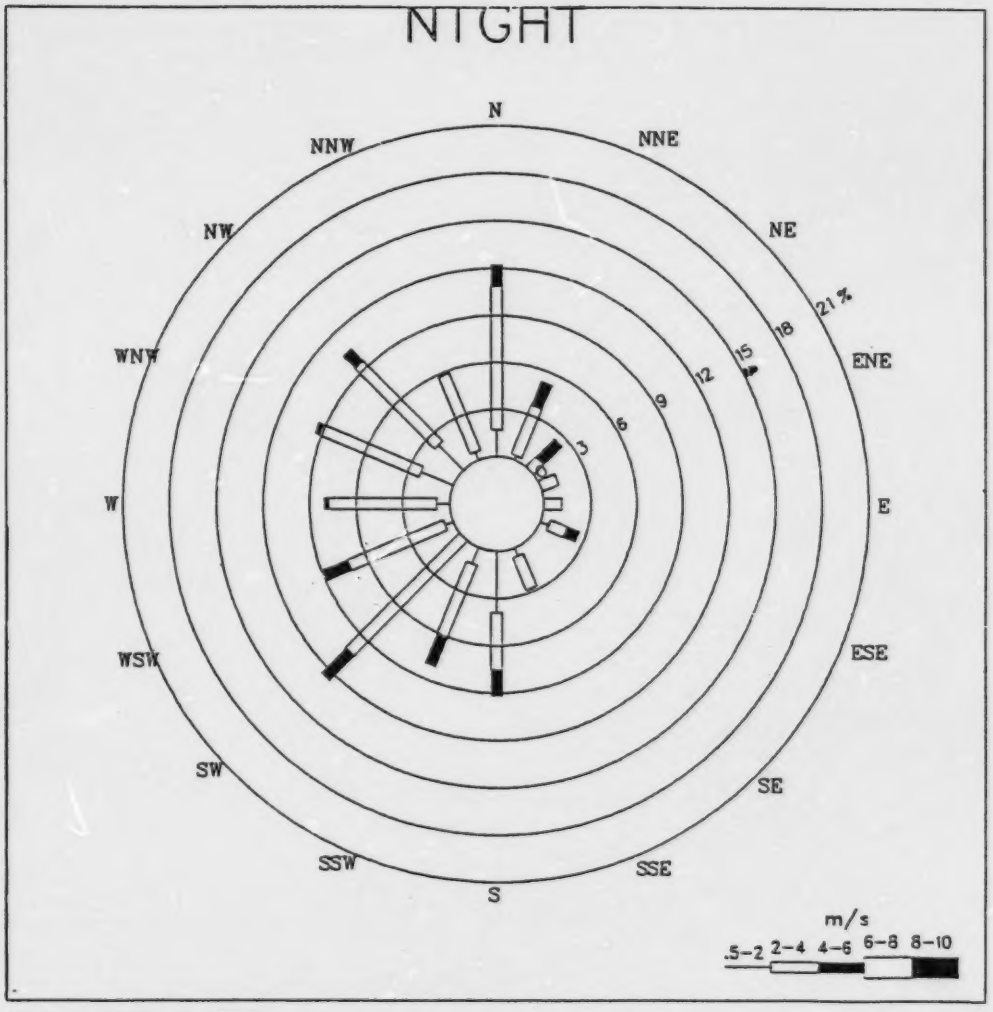


Figure 3. Average nighttime wind distribution during PAFS.

approximately from SW to NE. Hence, the PAFS station receptors should receive significant contributions from point sources both day and night. The nighttime wind rose also shows a strong northerly component; the nocturnal winds are evenly distributed from WSW to NW.

The frequencies of the six PG stability classes in the hourly meteorological data used in model evaluation are shown in Fig. 4. The slightly unstable (class C) cases during the day, and moderately stable (class F) cases during the night, occur frequently. There are roughly equal number of daytime and nighttime neutral cases. The frequencies of class B (moderately unstable) during day and class E (slightly stable) during night are also about equal.

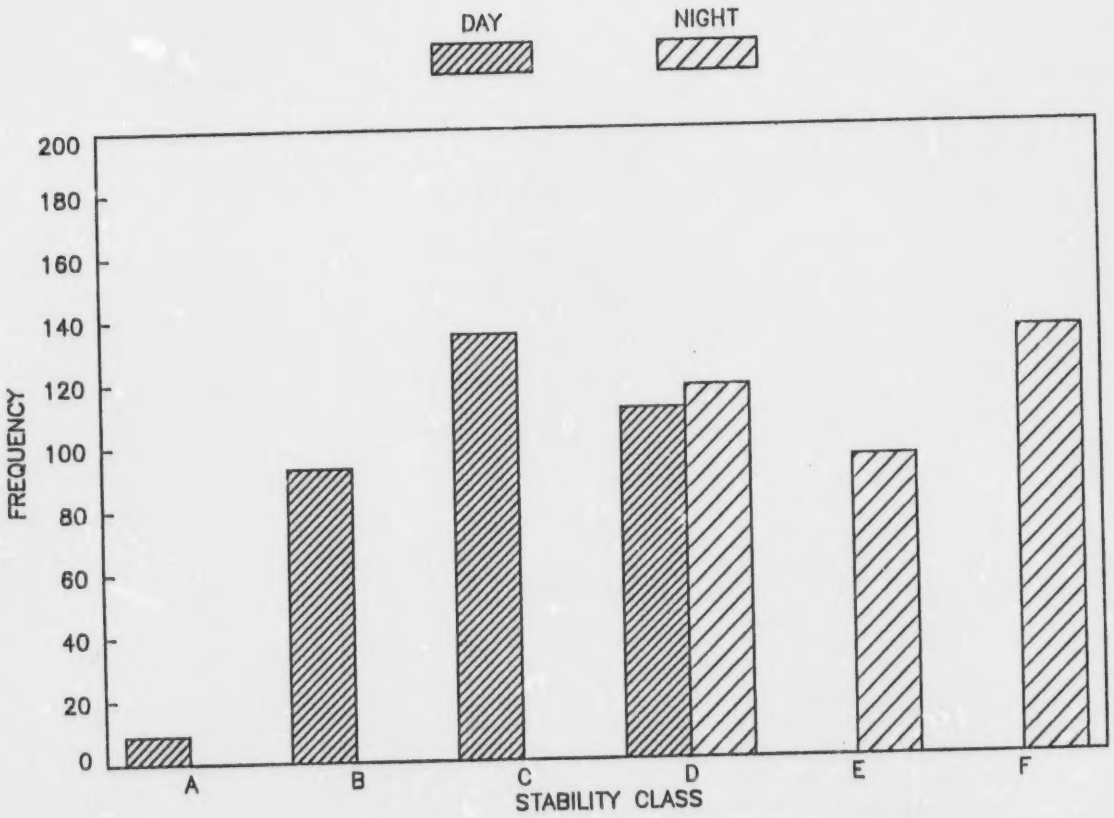


Figure 4. Frequencies (No. of hours) of PG stability classes during PAFS.

## SECTION 3

## MODEL EVALUATION

The details of the PEM-2 computer runs, input parameters, and statistical procedures of the model evaluation are discussed in this section.

### PEM-2 RUNS

The PEM-2 concentration predictions are evaluated against the measured concentrations of four pollutant species:

1) $SO_2$
2) Fine sulfate particles
3) FP total mass
4) CP total mass

The coarse sulfate concentrations could not be evaluated separately since coarse sulfate emissions are assumed to be zero in the PAFS inventory (see Section 2). The four species are calculated in two model runs as follows:

| Run | Pollutant-1 | Pollutant-2 | Note |
|---|---|---|---|
| I | $SO_2$ | Fine sulfate | Chemical transformation of $SO_2$ to fine sulfate is considered. |
| II | Fine mass | Coarse mass | No chemical coupling between the species. |

The fine total mass emissions in Run II also include the primary sulfate

particles. Though the emissions of the latter are assumed to consist only of fine particles, they obviously include some coarse (2.5 - 10 microns) sulfate particles as well since, for some point sources in the PAFS inventory, the primary sulfate emission rates exceed the corresponding fine total mass emission rates. Furthermore, the chemical transformation ($SO_2$ to fine sulfate) contribution to the calculated fine total mass concentration is ignored in Run II. These errors, however, are not expected to be serious for obtaining the urban-scale 12-hour average concentration estimates based on the entire inventory in this evaluation.

## Calculation Grid

The calculation grid consists of 32 x 32 cells, each a square of 2.5 km side. The southwest corner of the grid is set at XUTM = 444.5 km and YUTM = 4380 km, and the modeling domain covers 80 km x 80 km to incorporate the entire PAFS emission data. The calculation grid cell size is chosen to agree with the area source grid cell size of 2.5 km, so that emissions can be directly input to the model from the inventory data files. Figure 5 shows the calculation grid used for PEM-2 evaluation and the locations of the six PAFS stations.

For this evaluation, the maximum capacity of 50 area sources in PEM-2 is increased to accomodate all 289 area sources in the emission inventory. The PEM-2 program is also modified such that concentrations from point sources are calculated only at the four receptors (grid points) surrounding each PAFS station, and not at the rest of the receptors. This required calculation at only 24 out of a total of 1024 receptors, which resulted in a significant reduction in the computer run costs. The area source

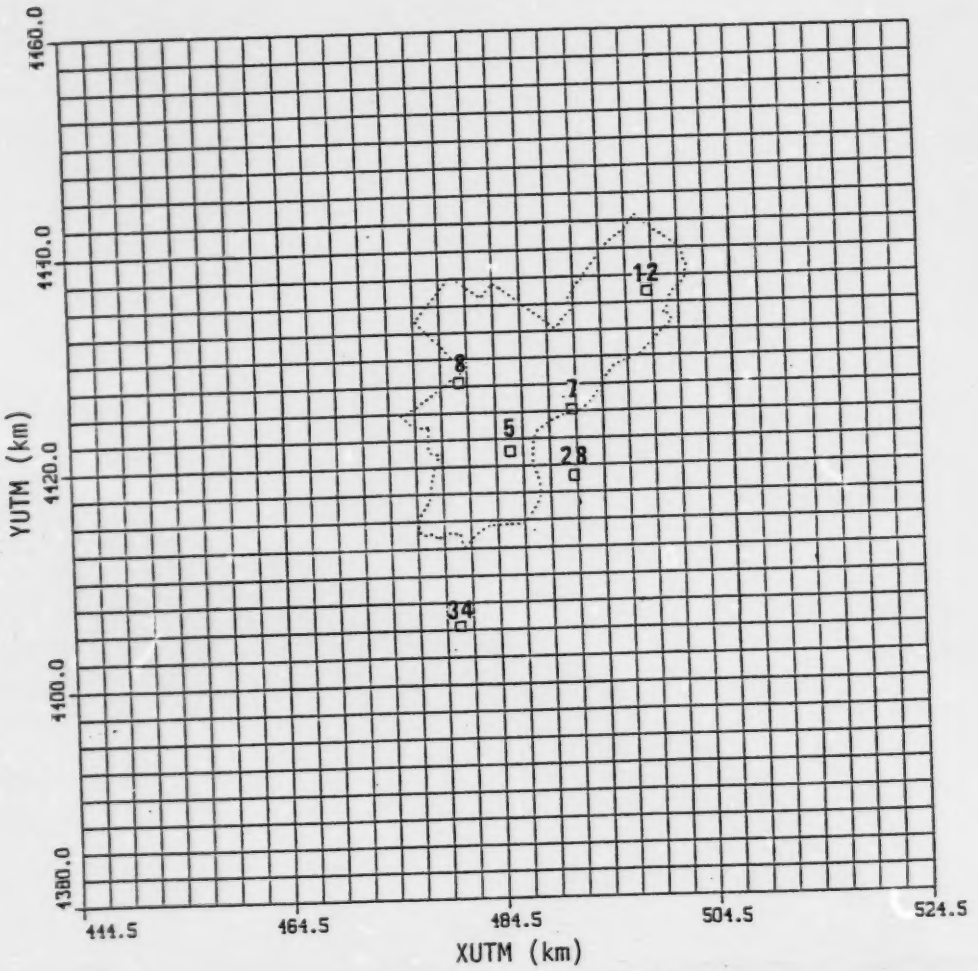


Figure 5. Calculation grid used for PEM-2 evaluation showing the locations of PAFS stations.

calculations did not include this modification to the program. For each of the area sources, the contributions to the concentrations at the nine affected receptors located within and immediately downwind of the source are calculated, as discussed by Rao (1985). The total concentration at each PAFS station is then determined as the weighted average of the corresponding values calculated at the four surrounding receptors.

A calculation grid cell size of 5 km side square is also tested in the evaluation. The results showed that, for the PAFS emissions inventory, the calculations are not very sensitive to this change in the grid cell size.

## Emission Data

The hourly emission data are scanned and point sources with emissions less than 1 g/s of $SO_2$ and 0.1 g/s of $SO_4$ are eliminated in order to reduce computer run costs. The emissions are analyzed for day-to-day as well as diurnal variability.

Figure 6 shows the variations of daily total (daytime + nighttime) $SO_2$ emissions from all of the point and area sources in the PAFS inventory during the evaluation period. Figure 7 shows a similar plot for daily total sulfate emissions. It can be seen that the point-source total emissions show large day-to-day variability; for example, $SO_2$ and sulfate emissions increase by roughly 50 percent from Day 17 to Day 18, and decrease by a similar amount from Day 22 to Day 23. Days 18 to 22 (August 2-6) are characterized by unusually large point-source emissions, most probably due to increased power demand for air-conditioning during the hot summer days. In contrast, the area-source total $SO_2$ and sulfate emissions

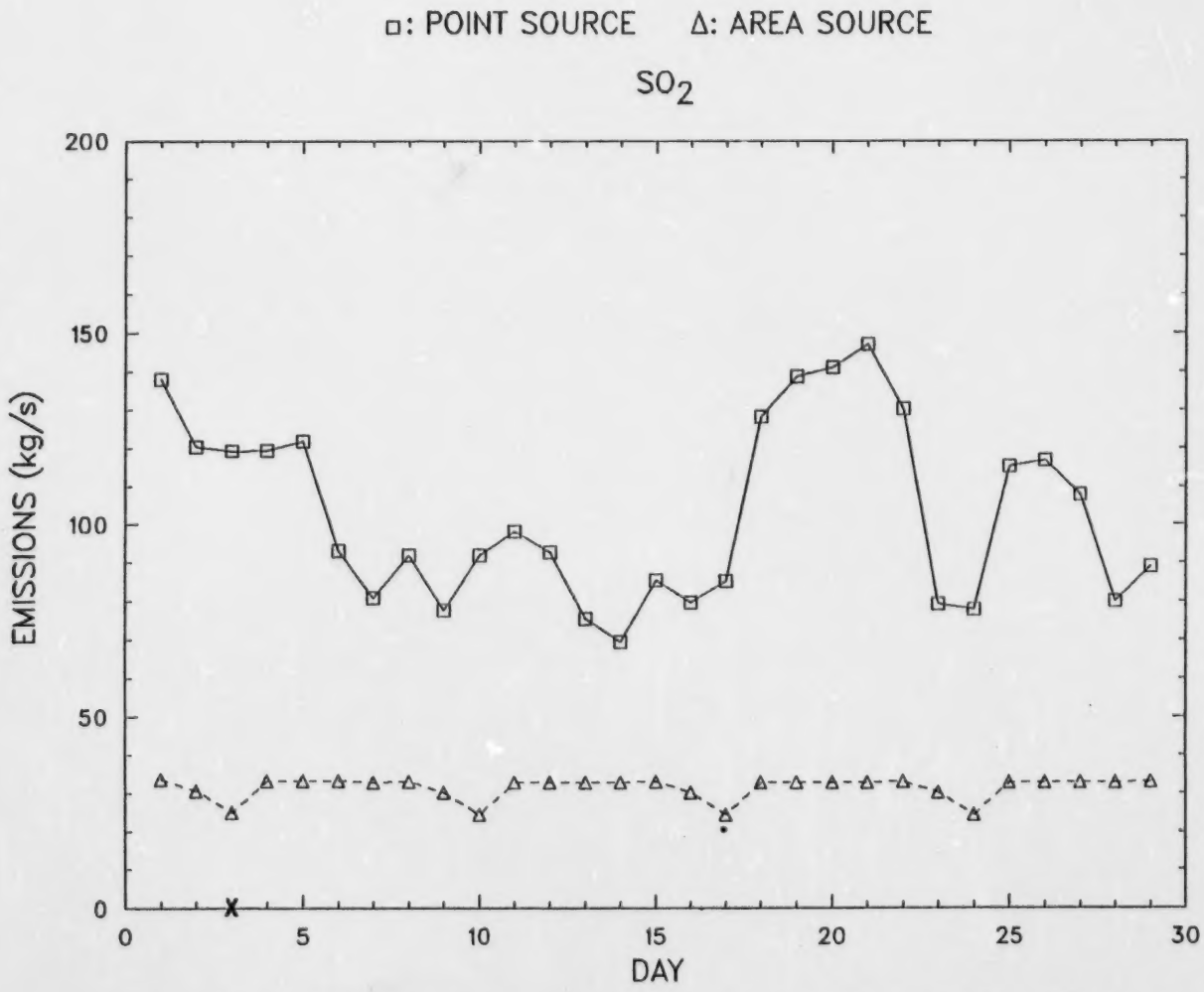


Figure 6. Variations of daily total (daytime + nighttime) $SO_2$ emissions from point and area sources in Philadelphia for the evaluation period. First Sunday of the PAFS period is denoted by X.

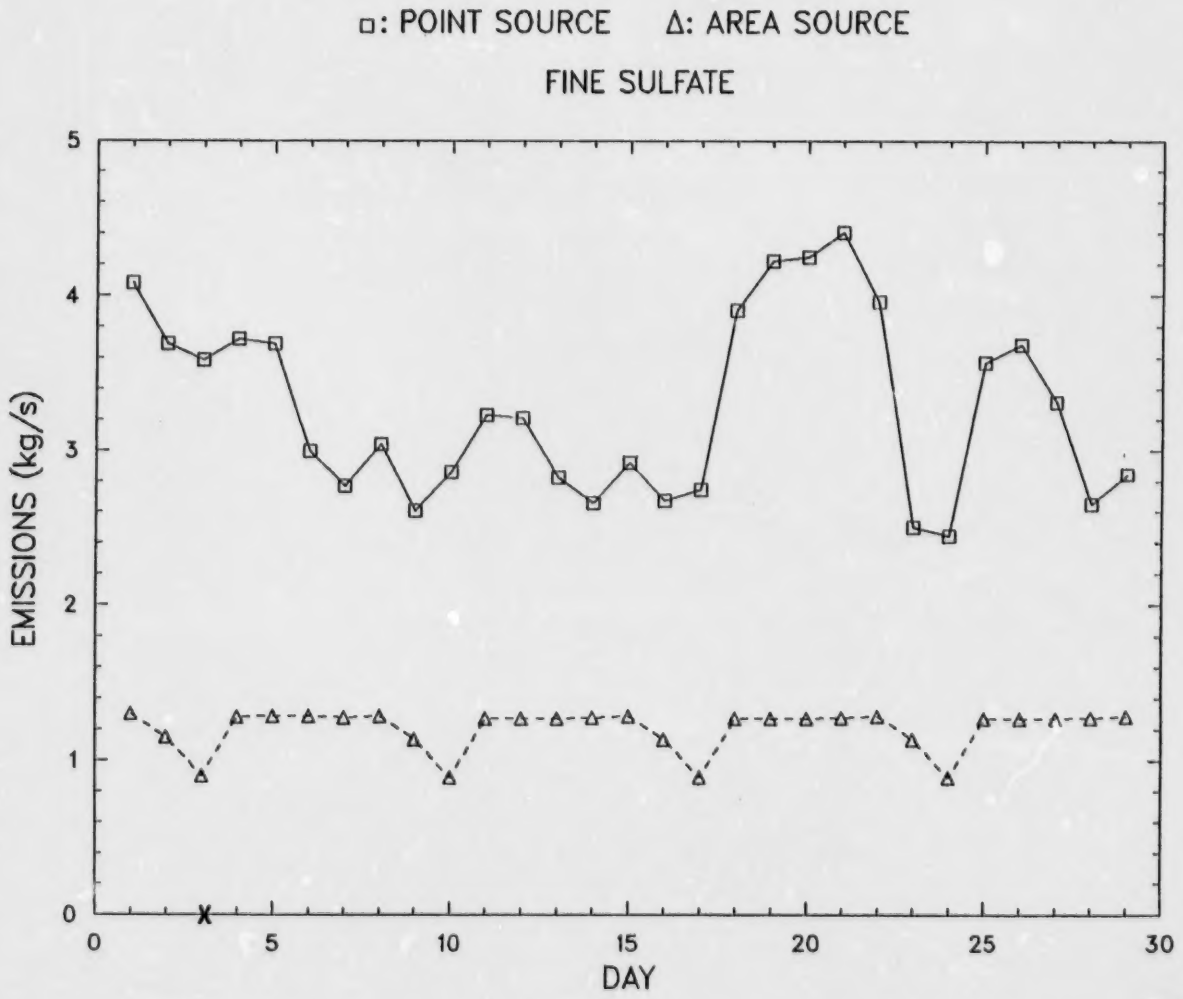


Figure 7. Same as in Fig. 6, except for sulfate emissions.

are constant during weekdays, and decrease during weekends to their minimum values on Sunday.

Figures 8 and 9 show variations of daily total (daytime + nighttime) emissions of FP and CP total mass, respectively. The point-source fine mass emissions show significant day-to-day variability during the evaluation period, while the coarse mass emissions do not vary much. The area source emissions of both fine and coarse mass show periodic variations, typically increasing slightly during weekdays to a maximum value on Friday, and decreasing during weekends to a minimum on Sunday. These variations are probably dictated by traffic patterns and fugitive particulate emissions from unpaved highways, and emissions from industrial and construction activities.

The diurnal variations of $SO_2$ and sulfate emissions from point and area sources in Philadelphia (averaged over the 29-day evaluation period) are shown in Figs. 10 and 11, respectively. The point-source emissions increase sharply after 7 a.m. to their daytime peak values and then decrease rapidly after 8 p.m. The area-source emissions also behave in a similar manner, though these values are much smaller than the point-source emissions. However, area sources dominate the daytime emissions of fine and coarse total mass as shown in Figs. 12 and 13, respectively. The total particulate emissions increase sharply from 5 a.m. to a daytime peak at 7 a.m., and decrease rapidly from a secondary peak at 4 p.m. Thus, these emissions strongly correlate with rush-hour traffic patterns and daytime industrial activity.

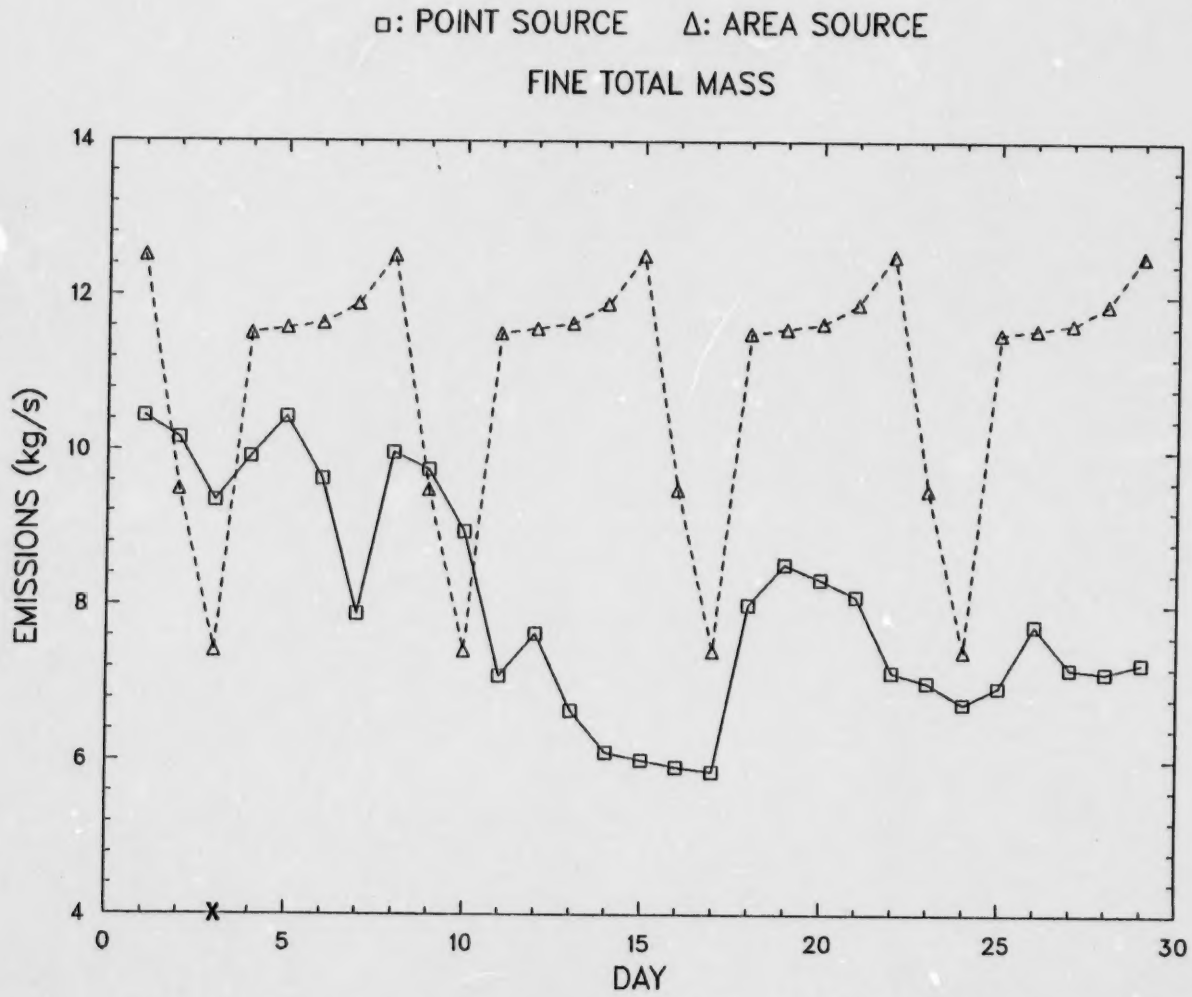


Figure 8. Same as in Fig. 6, except for fine total mass emissions.

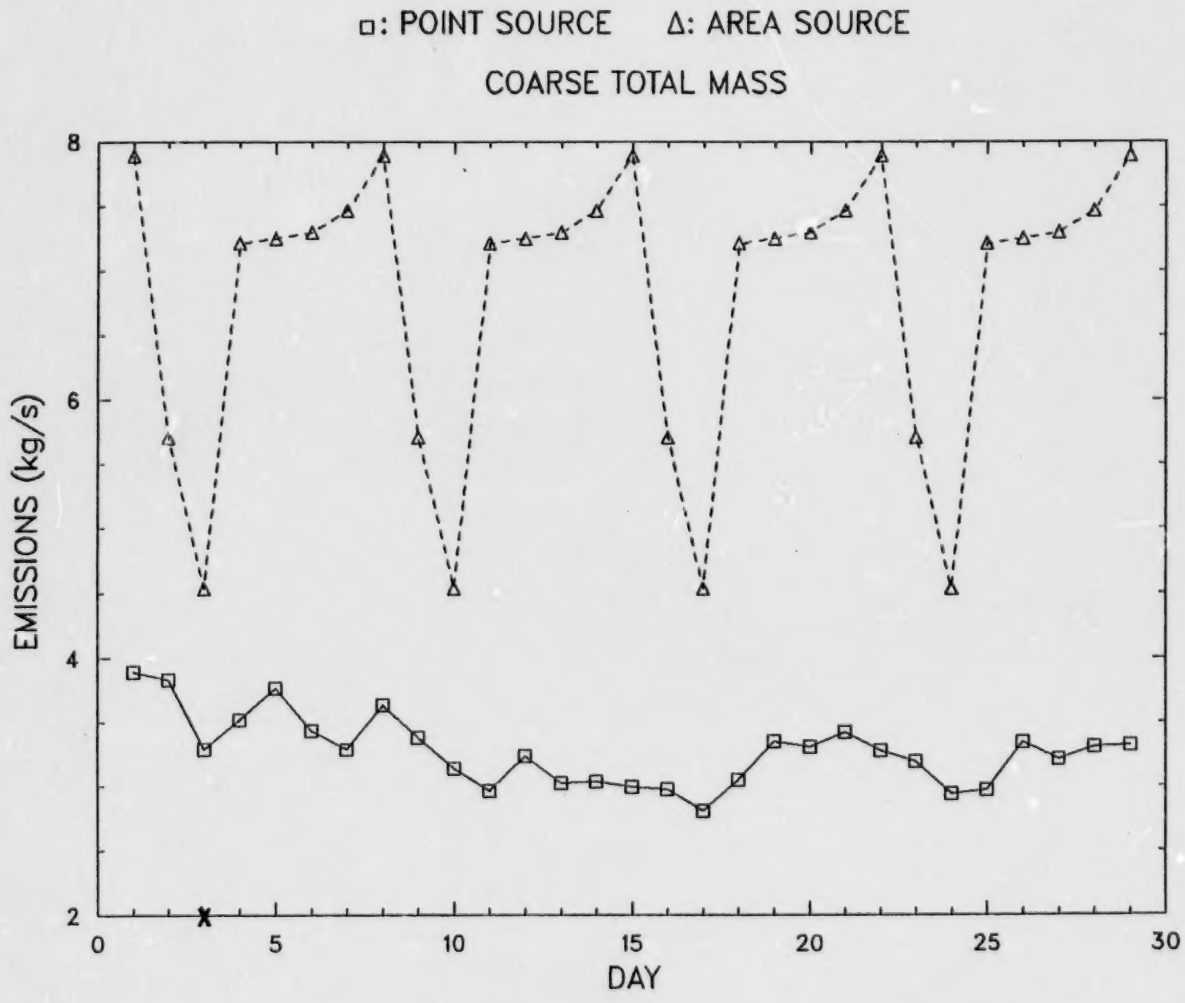


Figure 9. Same as in Fig. 6, except for coarse total mass emissions.

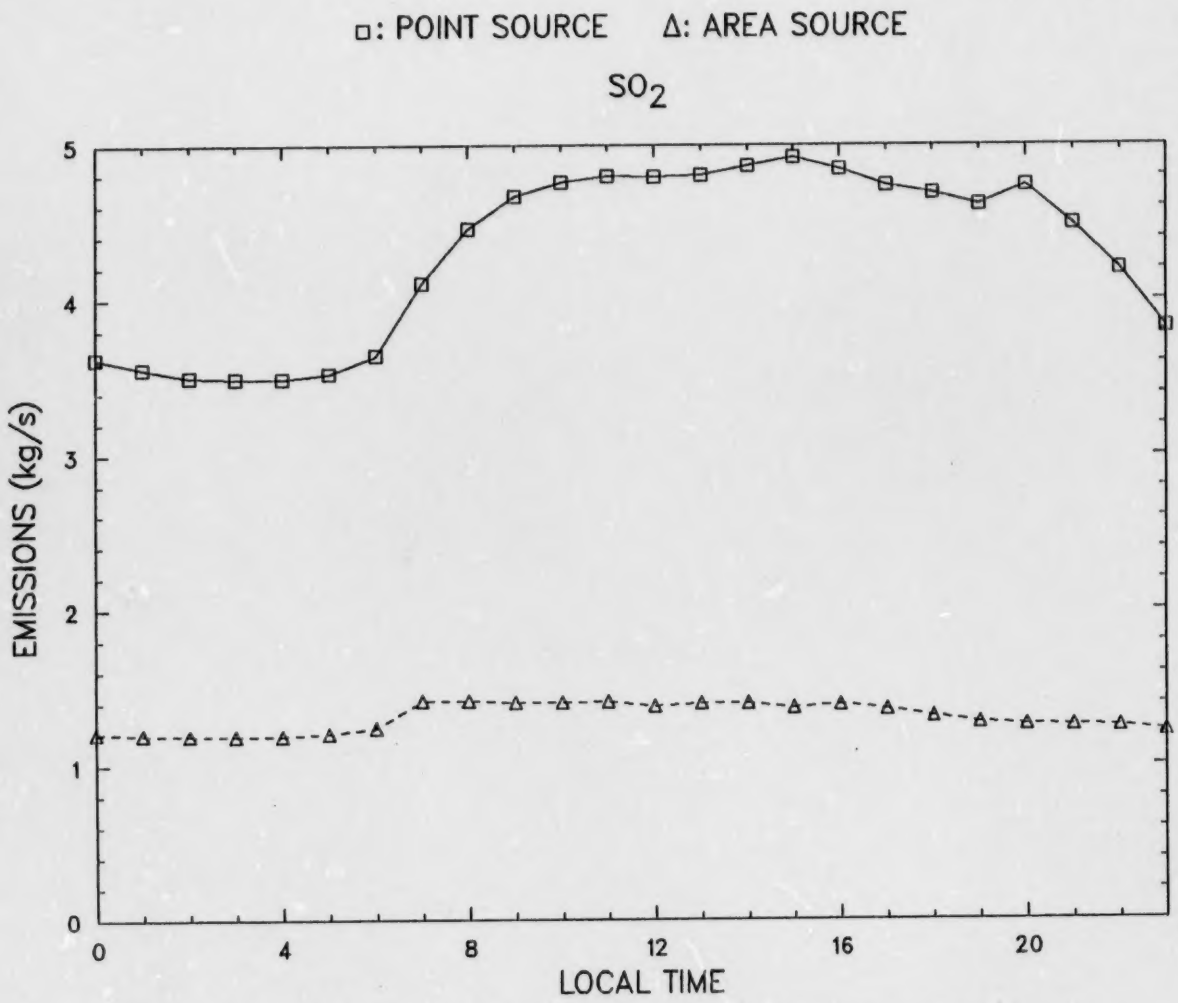


Figure 10. Diurnal variation of $SO_2$ emissions (averaged over the evaluation period) from point and area sources in Philadelphia.

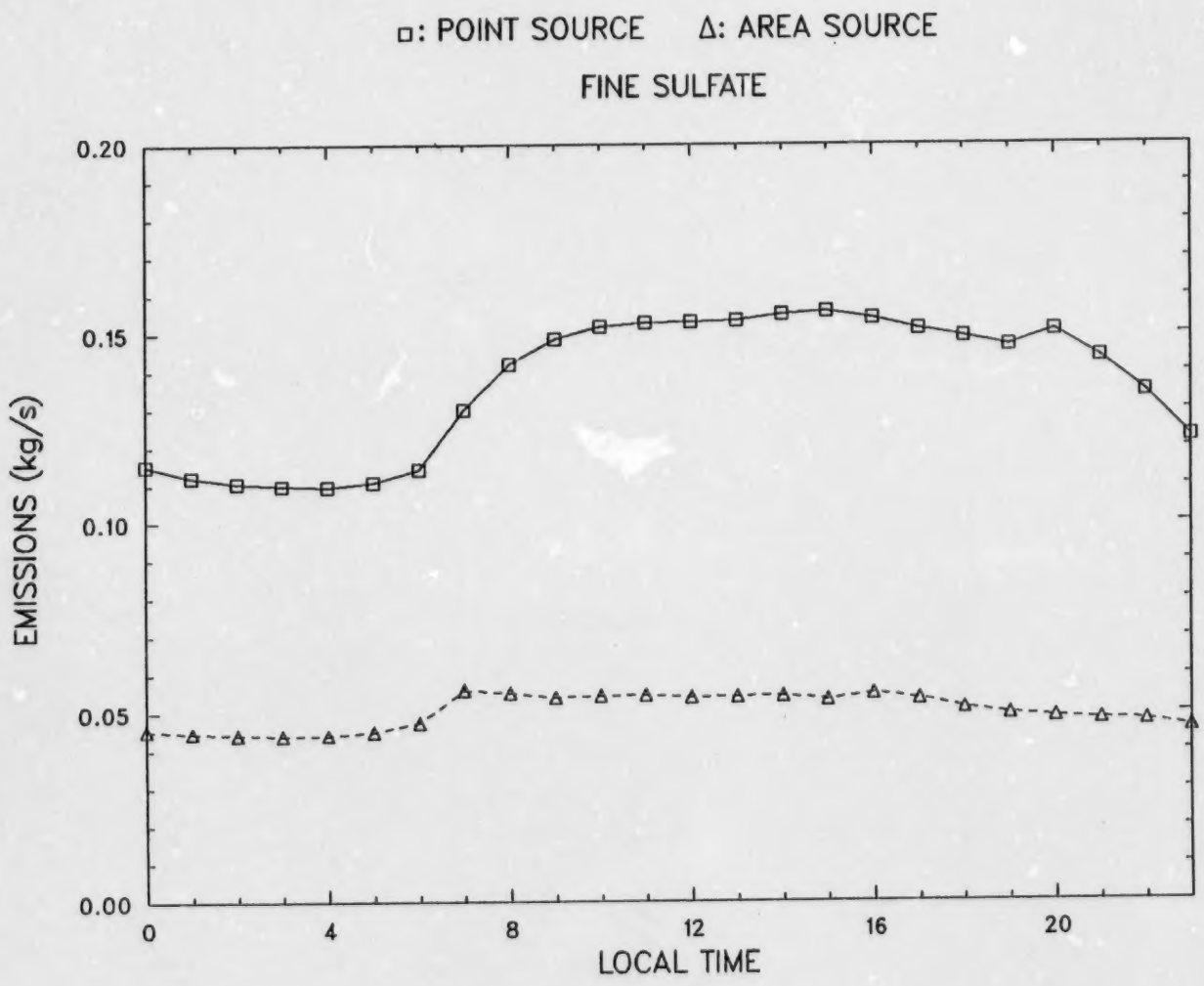


Figure 11. Same as in Fig. 10, except for sulfate emissions.

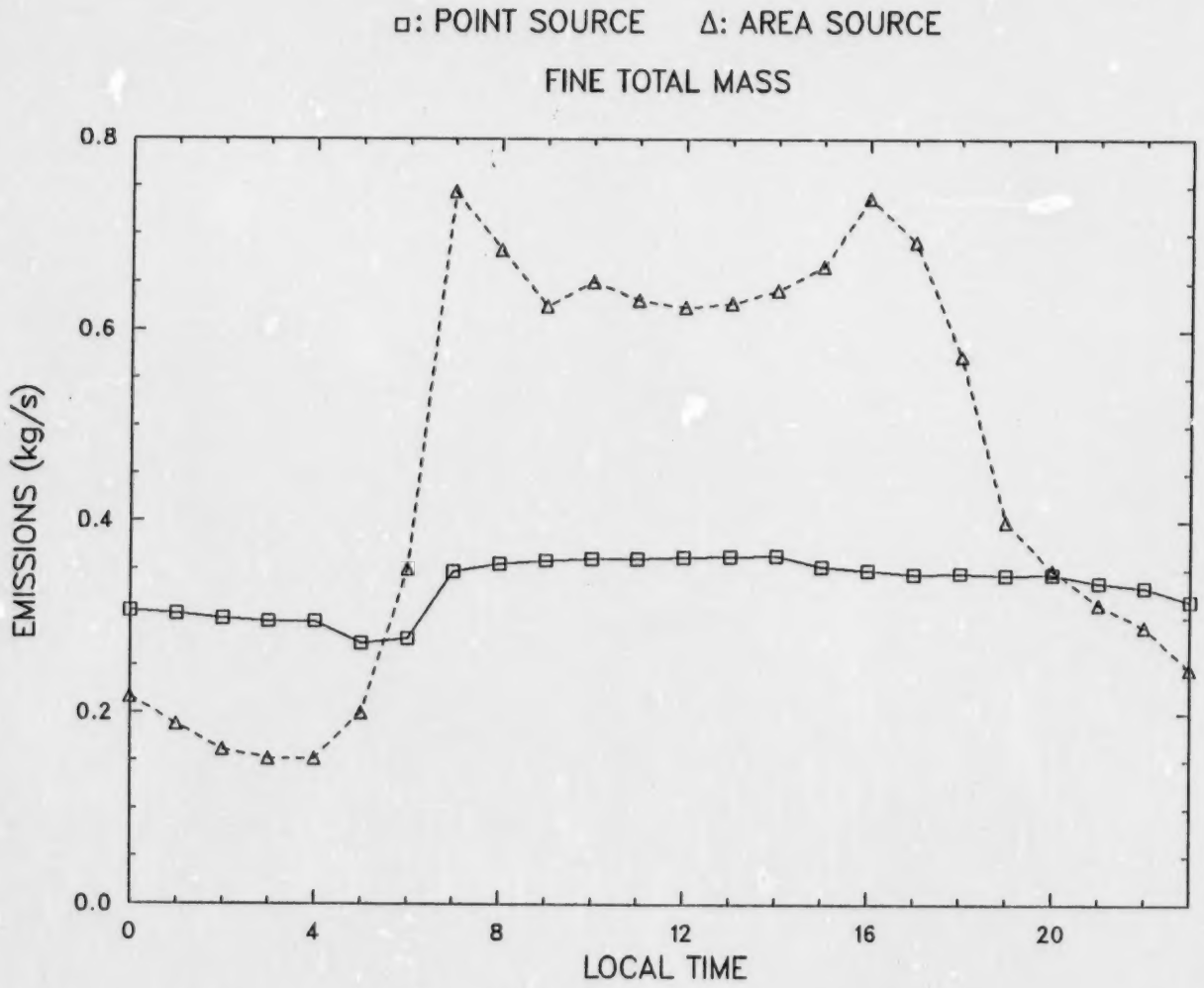


Figure 12. Same as in Fig. 10, except for fine total mass emissions.

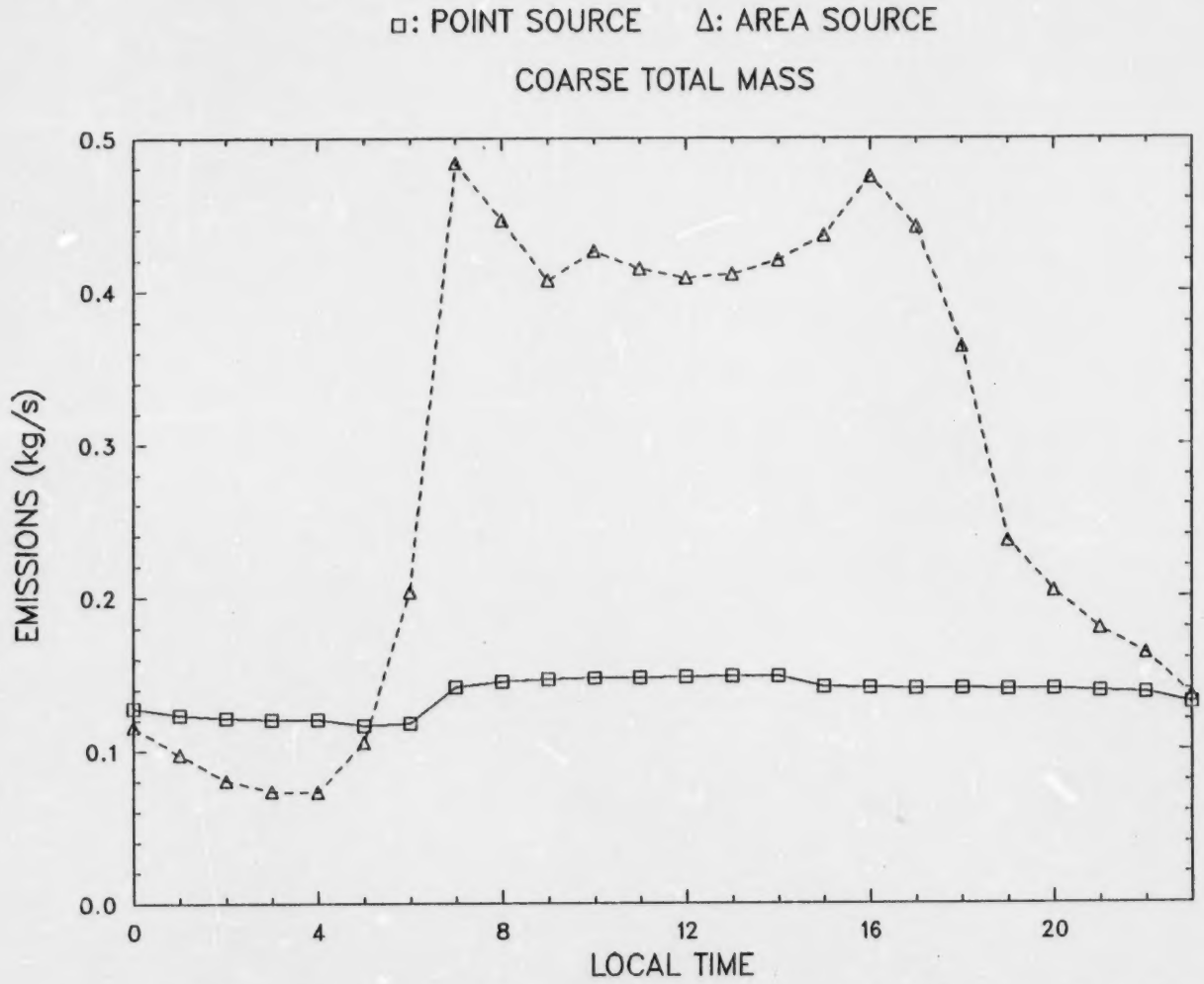


Figure 13. Same as in Fig. 10, except for coarse total mass emissions.

The total emission rates of the four pollutant species from point and area sources, averaged over the evaluation period and stratified by day and night, are shown in Table 2. It can be seen that point sources dominate the $SO_2$ and sulfate emissions. The area sources dominate the fine and coarse mass emissions during the day; however, the contributions of point and area sources are roughly equal at night.

TABLE 2

Average Daytime and Nighttime Total Emission Rates (kg/s) from Area and Point Sources in PAFS Inventory.

| Pollutant | Area Sources | Point Sources |
|---|---|---|
| | Daytime (6:00 a.m. - 6:00 p.m.) | |
| $SO_2$ | 16.665 | 56.425 |
| Sulfate | 0.650 | 1.797 |
| Fine Mass | 7.897 | 4.269 |
| Coarse Mass | 5.133 | 1.737 |
| | Nighttime (6:00 p.m. - 6:00 a.m.) | |
| $SO_2$ | 14.683 | 46.697 |
| Sulfate | 0.555 | 1.480 |
| Fine Mass | 3.021 | 3.724 |
| Coarse Mass | 1.668 | 1.536 |

Comparing this with a similar tabulation of total emissions for the RAPS study from Pendergrass and Rao (1984), we note that unlike in St. Louis,

area sources in Philadelphia are significant contributors of $SO_2$ and sulfate, and point-source contributions to fine and coarse total mass are very important.

Deposition and Sedimentation Rates

Rao (1983) discussed the specification of deposition and gravitational settling velocities ($V_d$ and W, respectively) in PEM-2. These parameters are varied, depending on the pollutant and time period of the run (day or night), as follows:

| Pollutant | $V_d$ (cm/s) | | W (cm/s) |
|---|---|---|---|
| | Day | Night | Day & Night |
| $SO_2$ | 3.0 | 2.0 | 0.0 |
| Fine sulfate | 0.2 | 0.1 | 0.0 |
| Fine mass | 0.2 | 0.1 | 0.0 |
| Coarse mass | 0.5 | 0.5 | 0.25 |

These values are based on typical magnitudes of deposition velocities quoted in literature for surfaces with large roughness and turbulence intensity such as the urban area. The dependence of the deposition velocities on the atmospheric stability and other meteorological conditions is simulated approximately by specifying smaller values at night than during the day.

The average daytime oxidation rates of $SO_2$ reported in literature (see, e.g., Pendergrass and Rao, 1984) for urban areas range from 2 to 16 percent per hour. A median value of 7 percent per hour for the rate of chemical transformation of $SO_2$ to fine sulfate is used in Run I of this evaluation

during day. The sulfate formation rates are smaller at night due to the absence of photochemical mechanisms. A constant transformation rate of 3 percent per hour is used for the nighttime runs in this study.

## Model Calculations

The PEM-2 is run with hourly data of meteorology and emissions to estimate the hourly concentrations. The output data are stored on a magnetic tape, and later summed and averaged to obtain 12-hour average (day and night) values. The model evaluation runs are made with the following technical options (see, Rao, 1985) in effect:

1) Wind-profile exponents option: NWPOPT = 0, standard values are used;
2) Stack-tip downwash option: NSTDWN = 0, downwash algorithm is used;
3) New plume-rise equations option: NPRISE = 1, new equations are used to estimate maximum rise of buoyancy-dominated plumes from point sources in unstable or neutral atmosphere;
4) New plume-penetration schemes option: NINPEN = 1, new schemes are used for estimating penetration of an elevated stable layer (capping unstable/neutral atmosphere) by buoyancy-dominated plumes from point sources.

The default values of atmospheric potential temperature gradients for E and F stability classes (0.02 and 0.035°C/m, respectively) are used in the plume rise equations under stable conditions. The area source emissions are assumed to be located at an effective height HAS = 10 m, which is a typical building height in urban areas. This value is kept constant for all area sources and species both day and night.

## Background Concentrations

The calculated 12-hour average sulfate, fine and coarse total mass concentrations, resulting only from the contributions of point and area sources to the receptors, are added to their respective background concentrations. The latter are determined as the lowest observed 12-hour average concentrations at one of the four PAFS stations 8, 12, 28, and 34 located in a generally upwind direction during the averaging period. Stations 5 and 7, which are located in the downtown urban area and have higher observed concentrations compared to the other stations, are not used for this background analysis. The background concentrations of $SO_2$ are assumed to be zero.

The method of determining the background concentrations as described above is rather subjective due to the small number of monitoring stations available. However, the background particulate concentrations play an important role in evaluating the model performance by comparing the calculated concentrations to their observed values. For example, the calculated fine mass concentrations directly attributable to the emissions in Philadelphia are in the range of 0 - 20 $\mu g/m^3$ with an average of about 5 $\mu g/m^3$, while the background fine mass concentrations average about 25 $\mu g/m^3$. The observed coarse mass concentrations at the stations are more variable than for the fine mass; this suggests that local contributions may be more important for coarse mass. The calculated average concentration of coarse mass resulting from local emissions is below 5 $\mu g/m^3$, while its background concentration is about 10 $\mu g/m^3$.

The station-to-station variations of the observed sulfate concentrations are small, with the background values averaging about 7 $\mu g/m^3$.

On the other hand, the sulfate concentration calculated from direct emissions and chemical transformation is below 2 $\mu g/m^3$. Therefore, the background concentrations of particulate species play an important role in this evaluation.

## EVALUATION STATISTICS

The recommendations of two workshops sponsored by the American Meteorological Society (AMS) to review the statistical approach to air quality model evaluation and model uncertainty are summarized by Fox (1981, 1984). Discussions and applications of these statistical methods can also be found elsewhere in the literature (see, e.g., Ruff, 1983; Rao et al., 1985).

The predicted and the corresponding observed concentrations are treated as pairs in this evaluation. Two general measures of performance are used here: (a) measures of difference which include the bias, variance, gross variability or root mean squared error, average absolute gross error, mean fractional error, and index of agreement; (b) measures of correlation including the correlation coefficient, slope, and intercept; estimates of the predicted concentrations from the regression analysis allow determination of the systematic and unsystematic parts of the mean squared error. The observed and predicted concentrations are analyzed and plotted with a standard SAS statistical and data-handling package (Ray, 1982).

In the discussion that follows, the observed concentrations are denoted by $O_i$ and the corresponding predicted concentrations (paired in space and time) are denoted by $P_i$. All sums are calculated over i = 1,2,-----,N,

where N is the number of observations. The means, $\overline{O}$ and $\overline{P}$, and standard deviations ($S_o$ and $S_p$) are computed as

$$\overline{O} = \frac{1}{N} \sum O_i \quad , \qquad \overline{P} = \frac{1}{N} \sum P_i \tag{1}$$

$$S_o = \left[ \frac{1}{N-1} \sum O_i'^2 \right]^{1/2} , \qquad S_p = \left[ \frac{1}{N-1} \sum P_i'^2 \right]^{1/2} \tag{2}$$

where $$O_i' = O_i - \overline{O} \quad , \qquad \sum O_i' = 0 \tag{3}$$

and $$P_i' = P_i - \overline{P} \quad , \qquad \sum P_i' = 0 \tag{4}$$

The mean and standard deviation of the ratios, $P_i/O_i$ , between the predicted and its associated observed value are also computed.

(a) Measures of Difference

Differences (residuals) are based on the observed and calculated concentrations such that

$$D_i = O_i - P_i \tag{5}$$

A negative residual indicates model overprediction and vice versa. The bias $\overline{D}$, which is the first moment of the distribution of differences, is defined as

$$\overline{D} = \overline{O} - \overline{P} = \frac{1}{N} \sum D_i \tag{6}$$

This is a measure of the overall bias of the model in predicting pollutant concentrations.

The average absolute gross error is defined as

$$\overline{|D|} = \frac{1}{N} \sum |D_i| \tag{7}$$

This measure of the absolute size of the error is less affected by the removal of outliers in the data than the root mean square error (RMSE). The estimated variance, which is the second moment of the distribution of differences, is calculated from

$$S_d^2 = \frac{1}{N-1} \sum D_i'^2$$

$$D_i' = D_i - \overline{D} \quad , \qquad \sum D_i' = 0 \tag{8}$$

where $S_d$ is the standard deviation. The variance is a measure of noise in the data. The RMSE, which is a measure of the actual size of the error produced by the model, is computed from

$$\text{RMSE} = \left[ \left( \frac{N-1}{N} \right) S_d^2 + \overline{D}^{\,2} \right]^{1/2} \tag{9}$$

The mean fractional error (MFE), which determines the model's overall bias to underpredict or overpredict the concentrations, is given by

$$\text{MFE} = \frac{1}{N} \sum \frac{D_i}{\left[ (O_i + P_i)/2 \right]^{1/2}} \tag{10}$$

For normally distributed variables, the bias has a normal distribution while the variance $S_d^2$ has a chi-squared distribution. The mean square error has a compound distribution. If the distributions of the predicted and observed concentrations are the same, then it is reasonable to assume that the differences are normally distributed with a zero mean and a constant variance.

The index of agreement is a measure of the degree to which the observed variable is accurately estimated by the calculated variable. This is not a measure of correlation, but rather a measure of the degree to which the model predictions are error-free. At the same time, it is a standardized measure so that cross-comparison of its magnitude for different models, or a model's performance at different receptor locations or under different atmospheric conditions, can be made. The index of agreement, d, is expressed as

$$d = 1 - \frac{\sum D_i^2}{\sum \left[ | P_i - \overline{O} | + | O_i' | \right]^2} \qquad (11)$$

Thus, d specifies the degree to which the observed deviations about $\overline{O}$ correspond, both in magnitude and sign, to the predicted deviations from $\overline{O}$. It is assumed that the parts of the magnitudes of $P_i$ and $O_i$ that are equivalent to $\overline{O}$ are not in error since $\overline{O}$ is considered to be error-free. All the potential for error is therefore assumed to be contained in the deviations of $P_i$ and $O_i$ from $\overline{O}$.

(b) Measures of Correlation

For each pollutant, a scattergram of predicted (on the ordinate) versus observed (on the abscissa) concentrations is plotted, and linear regression analysis is performed to determine a correlation coefficient (R), slope (b), and intercept (a), as follows:

$$R = \frac{\sum (O_i' \cdot P_i')}{\left[ \sum O_i'^2 \quad \sum P_i'^2 \right]^{1/2}} \qquad (12)$$

$$b = \frac{\sum (O_i' \cdot P_i')}{\sum O_i'^2} \quad , \qquad a = \overline{P} - b\,\overline{O} \tag{13}$$

The estimate of the predicted concentration, $\hat{P}_i$, is then given by

$$\hat{P}_i = a + b\,O_i \tag{14}$$

The unsystematic and systematic parts of the mean squared error (MSE) are computed as follows:

$$MSE(u) = \frac{1}{N} \sum (P_i - \hat{P}_i)^2 \tag{15}$$

$$MSE(s) = \frac{1}{N} \sum (\hat{P}_i - O_i)^2 \tag{16}$$

These new measures illuminating the sources or types of errors can be helpful in refining a model. When the MSE is largely systematic, further refinement in the model may be necessary in order to minimize the MSE so that the model can predict at its maximum possible accuracy. On the other hand, if MSE is largely unsystematic, the model is probably as good as it can be, and may not require major modifications. For each species, the complementary ratios MSE(u)/MSE and MSE(s)/MSE are computed and expressed as percentages.

# SECTION 4

## RESULTS AND DISCUSSION

The PEM-2 is evaluated using 29 days of data from Philadelphia for four pollutant species: $SO_2$, sulfate, fine and coarse mass. Only $SO_2$ concentrations are measured hourly; the particulate data are 12-hour averages. The evaluation results comparing the model's concentration estimates to the corresponding observed values are presented and discussed in this section.

### SULFUR DIOXIDE

The hourly $SO_2$ concentration data provide a demanding test of short term models such as PEM-2, especially since the background $SO_2$ concentrations are assumed to be zero. Figure 14 shows a comparison of the calculated and observed diurnal variations of $SO_2$ concentrations (averaged over the evaluation period) at Station 5. Similar plots for the other monitoring stations are shown in Figs. 15 to 19.

At all stations, the calculated and observed concentrations are closer during daytime than at night. The model generally overpredicts the hourly average concentrations at night.

A significant overestimation of $SO_2$ concentrations by the model at Stations 5 and 7, and also 28 to a somewhat lesser extent, is evident when compared with the evaluation results at other stations. The overpredic-

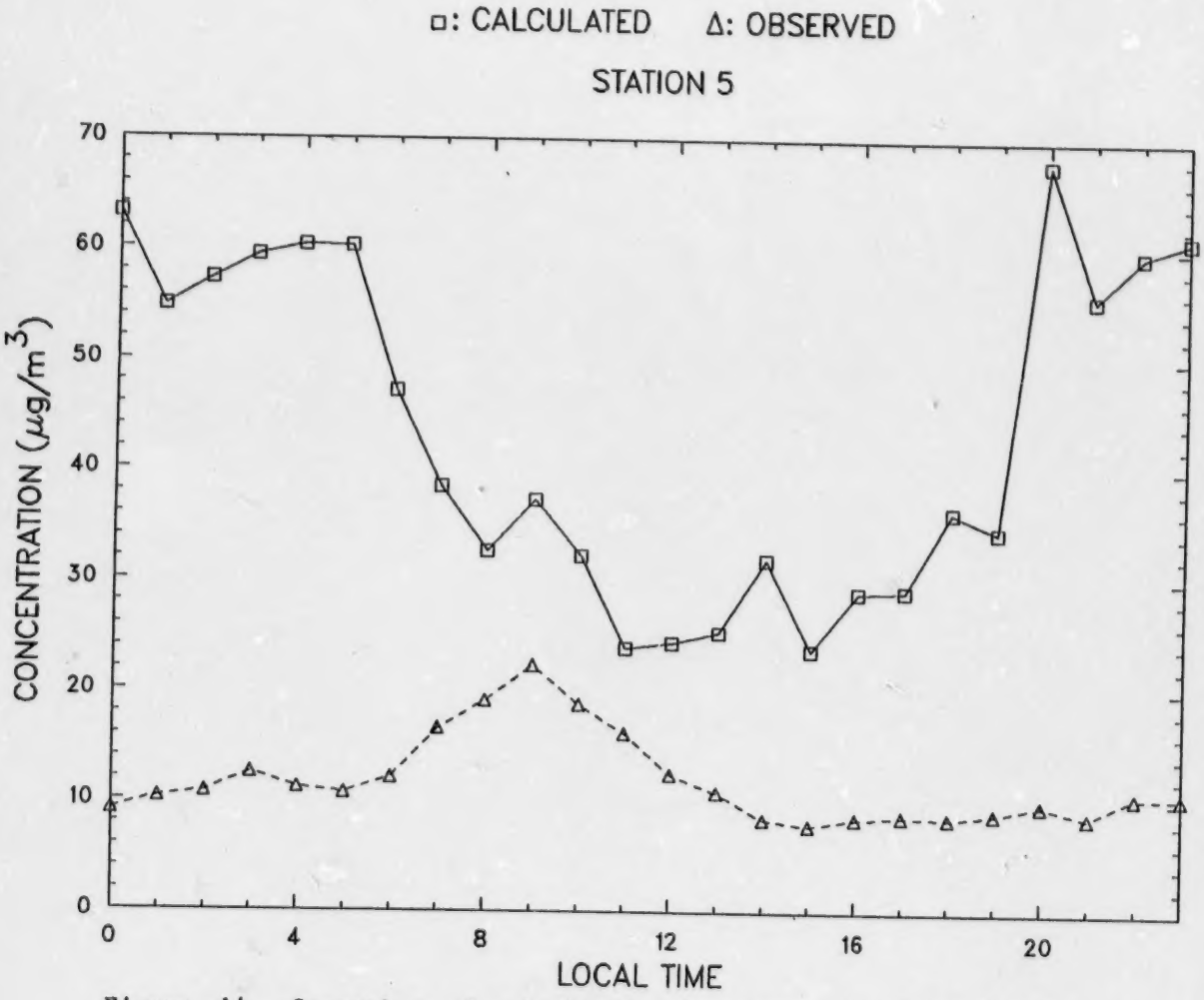


Figure 14. Comparison of calculated and observed diurnal variations of $SO_2$ concentrations (averaged over the evaluation period) at Station 5.

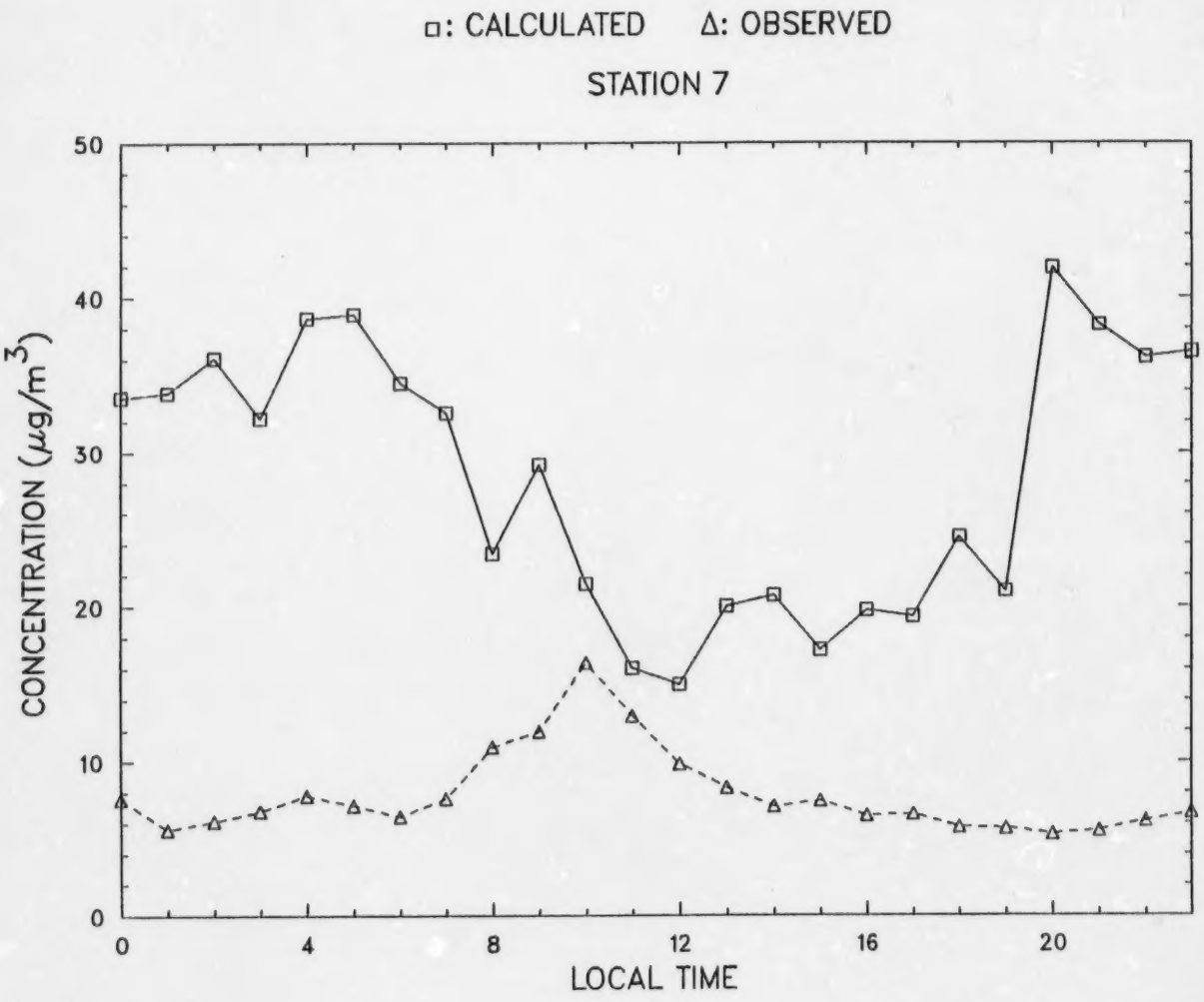


Figure 15. Same as in Fig. 14, except at Station 7.

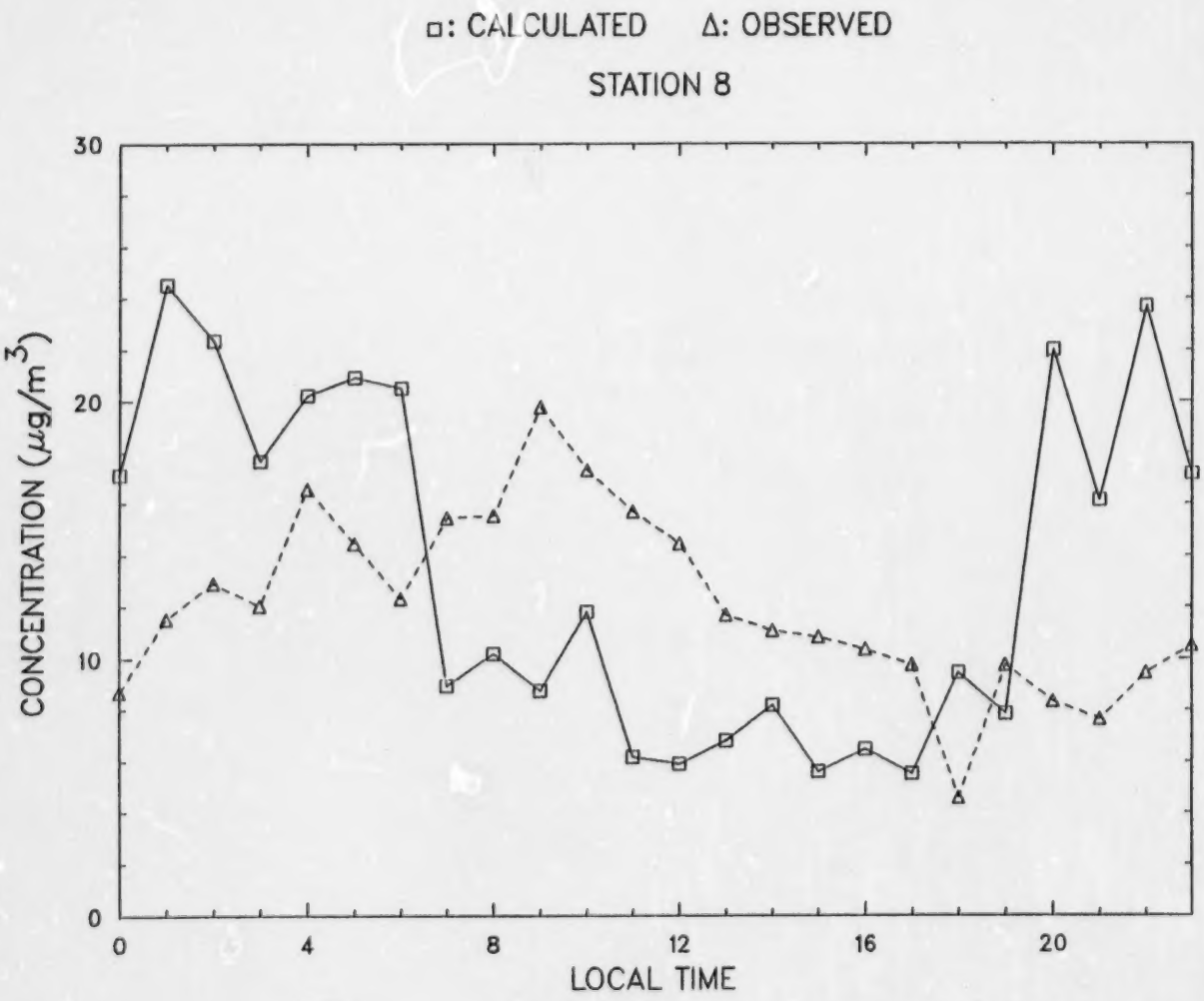


Figure 16. Same as in Fig. 14, except at Station 8.

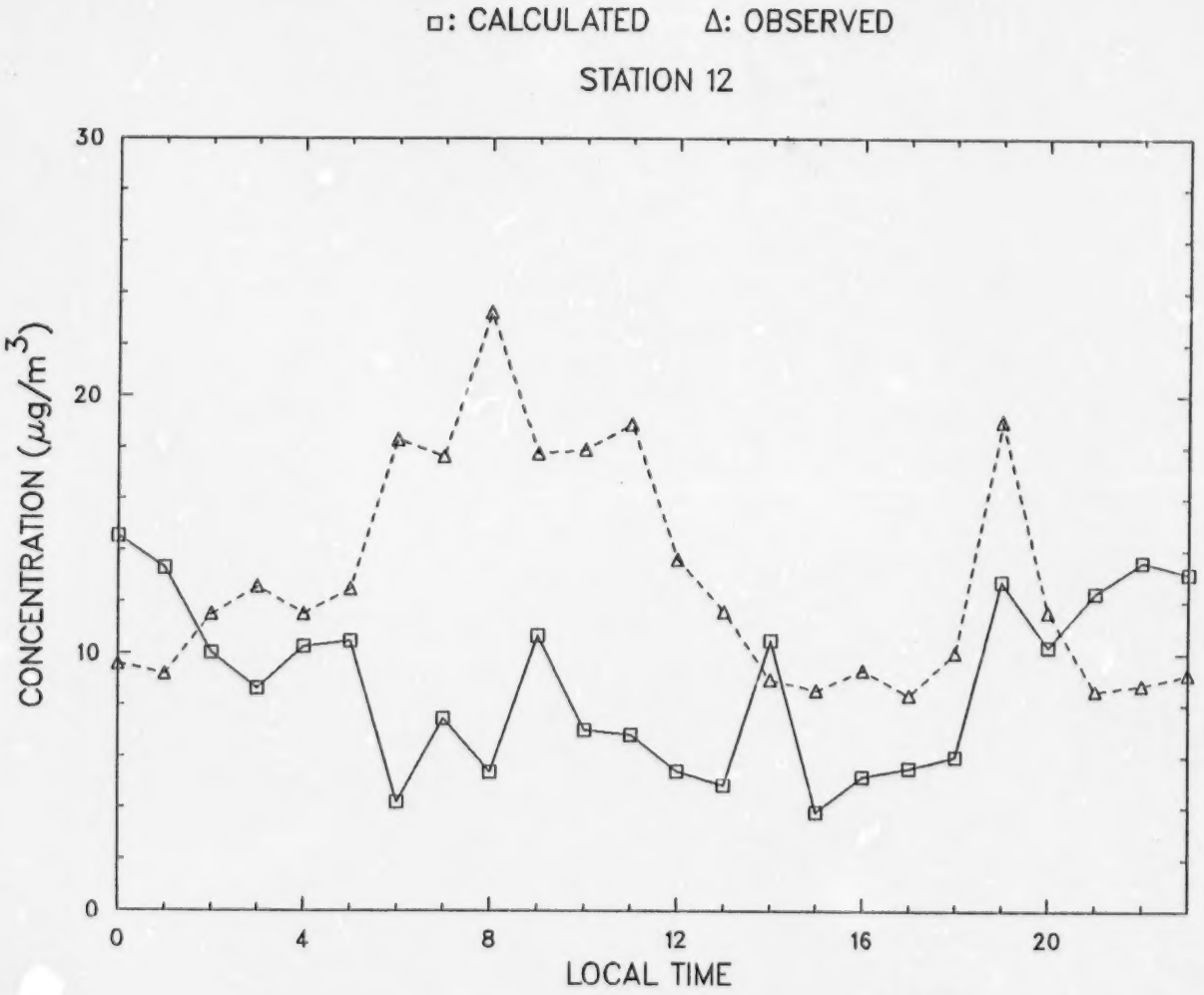


Figure 17. Same as in Fig. 14, except at Station 12.

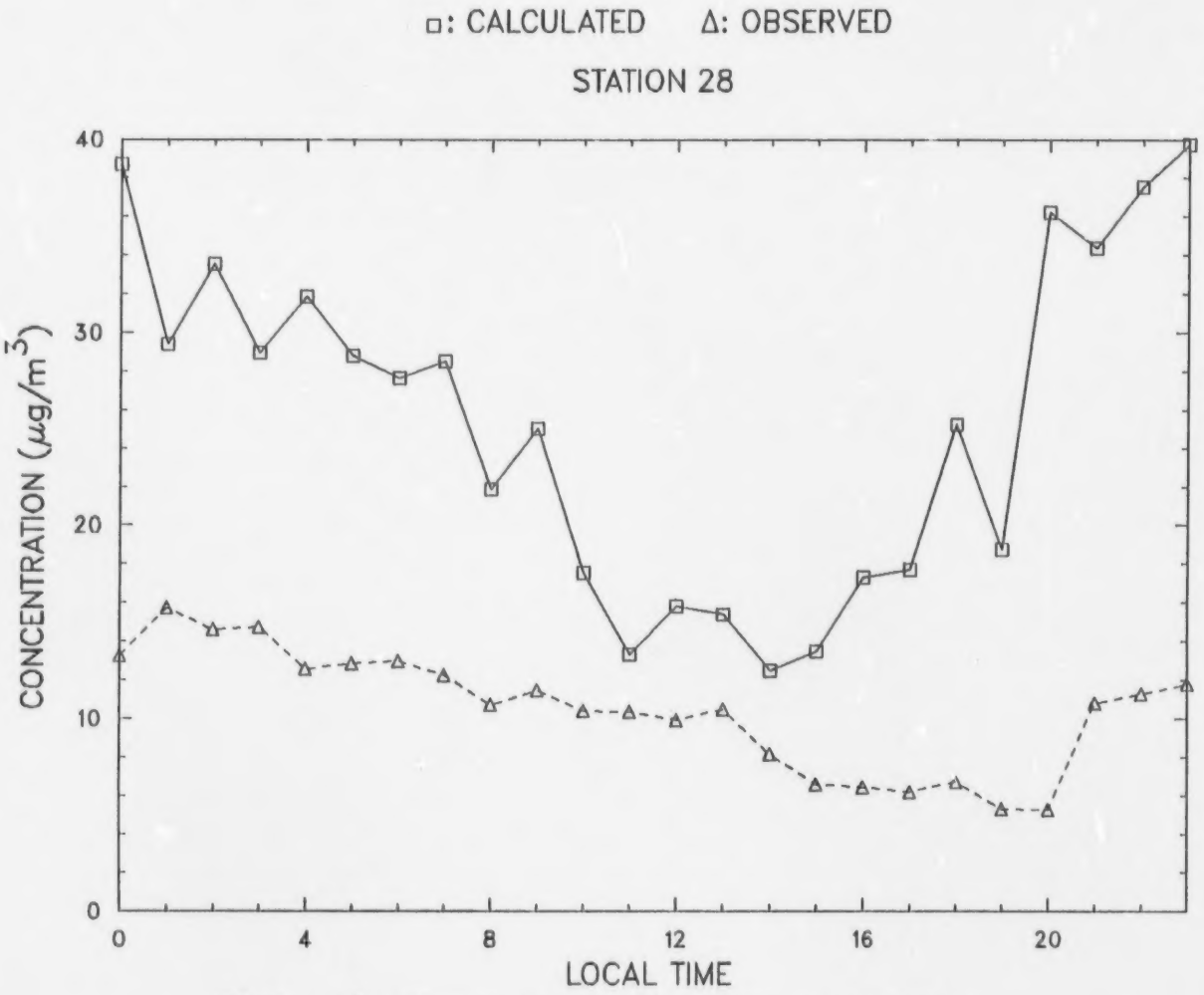


Figure 18. Same as in Fig. 14, except at Station 28.

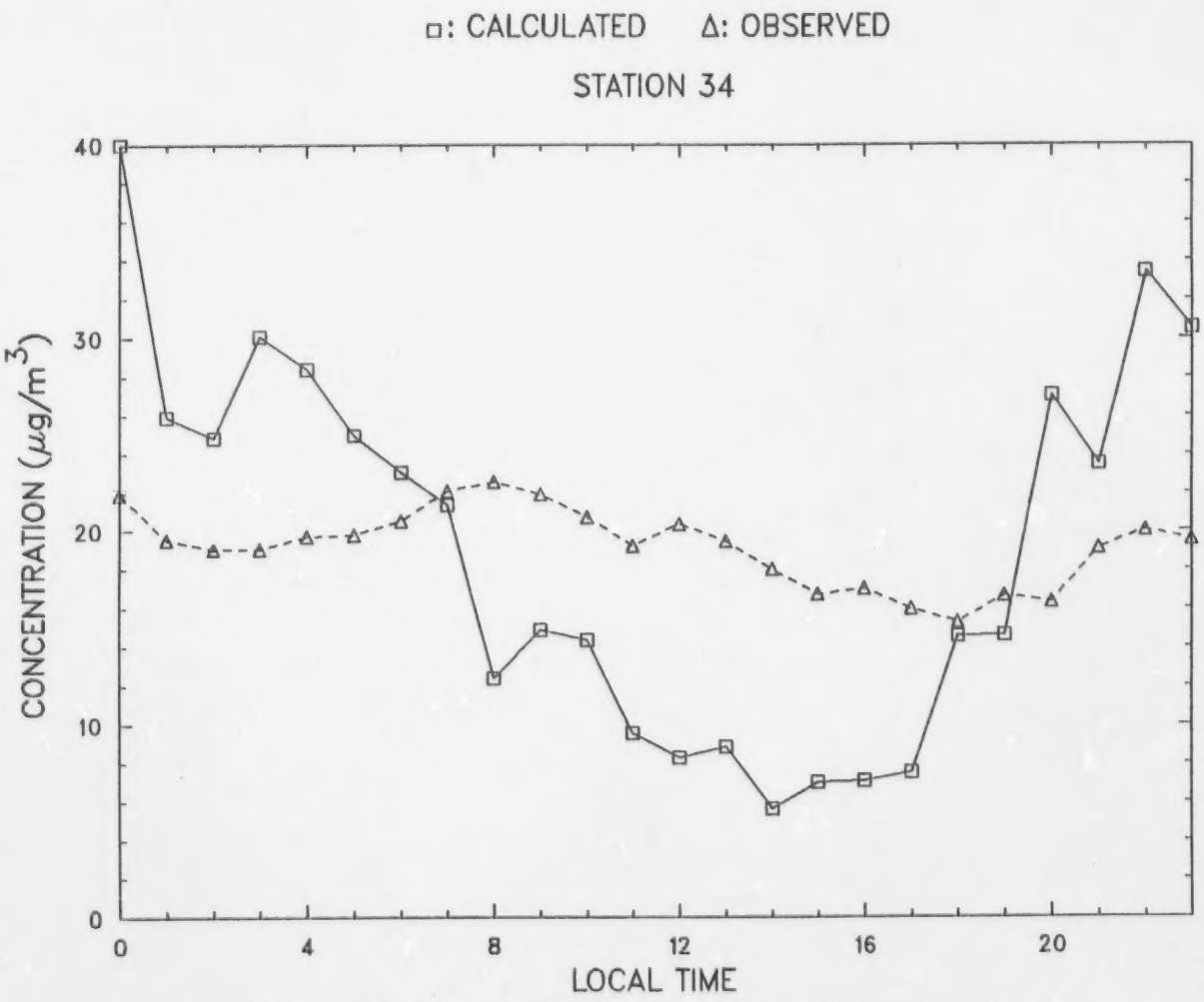


Figure 19. Same as in Fig. 14, except at Station 34.

tions at these stations during nighttime are more severe than during daytime. The emission sources in Philadelphia area are located roughly along an axis from southwest corner to northeast corner of the full calculation grid. Stations 5, 7, and 28 are located in the region of major area source emissions, and surrounded by many point sources. On the other hand, Stations 8, 12, and 34 are located away from the region of high area source emissions and may be impacted mostly by the point sources. At these stations, the model underestimates the observed concentrations during day, and overestimates during night.

From the above, it is clear that the model overprediction results mostly due to errors in estimating concentrations from the urban area sources using the narrow plume hypothesis and other simplifying assumptions (see, Rao, 1983). Uncertainties in the area-source emission conditions such as source height, plume rise, and building wake effects also contribute to these errors. In general, the isolated point source emission inventories are better defined and documented than those of the distributed urban area sources. The pattern of urban model estimates being highest under stable (nighttime) conditions and lower under unstable (daytime) conditions is attributed by Turner and Irwin (1985) to the errors in modeling low-level sources.

The plots show that the observed concentration reaches a maximum about 2 to 3 hours after the morning transition when the stratification changes from stable to neutral or unstable. The fumigation process which brings down the elevated plume from above the surface-based inversion may partly account for the peaks observed soon after sunrise (Rao et al., 1985). Though PEM-2 does not treat the fumigation process, the model simulates

these peaks quite well; this suggests that the observed peak concentrations may be related to the increases in $SO_2$ emissions in the morning (shown in Fig. 10).

Figure 20 shows a comparison of the calculated and observed 12-hour average $SO_2$ concentrations for the 29 evaluation days. This scatterplot is a composite of all (both day and night) paired comparisons at the six PAFS stations. The compared range of concentrations extends from 7.8 $\mu g/m^3$, which approximates the instrument accuracy, to a cutoff value of 57 $\mu g/m^3$ corresponding to 2.5 times the standard deviation, $S_p$. A linear regression fit, with a slope of 0.33 and an intercept of 17, is also shown in the figure.

Table 3 summarizes the model evaluation statistics for $SO_2$ for the total, day, and night paired data comparisons. The mean and standard deviation of the ratios $P_i/O_i$ are 1.51 and 1.66, respectively. Of particular interest is the better performance of the model during the day than at night. The index of agreement (0.43 for daytime and 0.21 for nighttime) suggests that PEM-2 calculations of $SO_2$ concentrations are more accurate during the daytime than at night.

The differences $D_i$ between observed and predicted concentrations are plotted in Fig. 21 against the observed concentrations. There is a tendency for the model to overpredict observed concentrations less than 25 $\mu g/m^3$. The bias D of -5.71 $\mu g/m^3$ indicates that PEM-2 overpredicts $SO_2$ concentrations on the average. This overprediction is mostly due to the nighttime cases for which the bias is -12.63 $\mu g/m^3$; the daytime $SO_2$ concentrations are slightly underpredicted. Because of the smaller diffusivities and mixing depths, the nighttime GLC may result mostly from

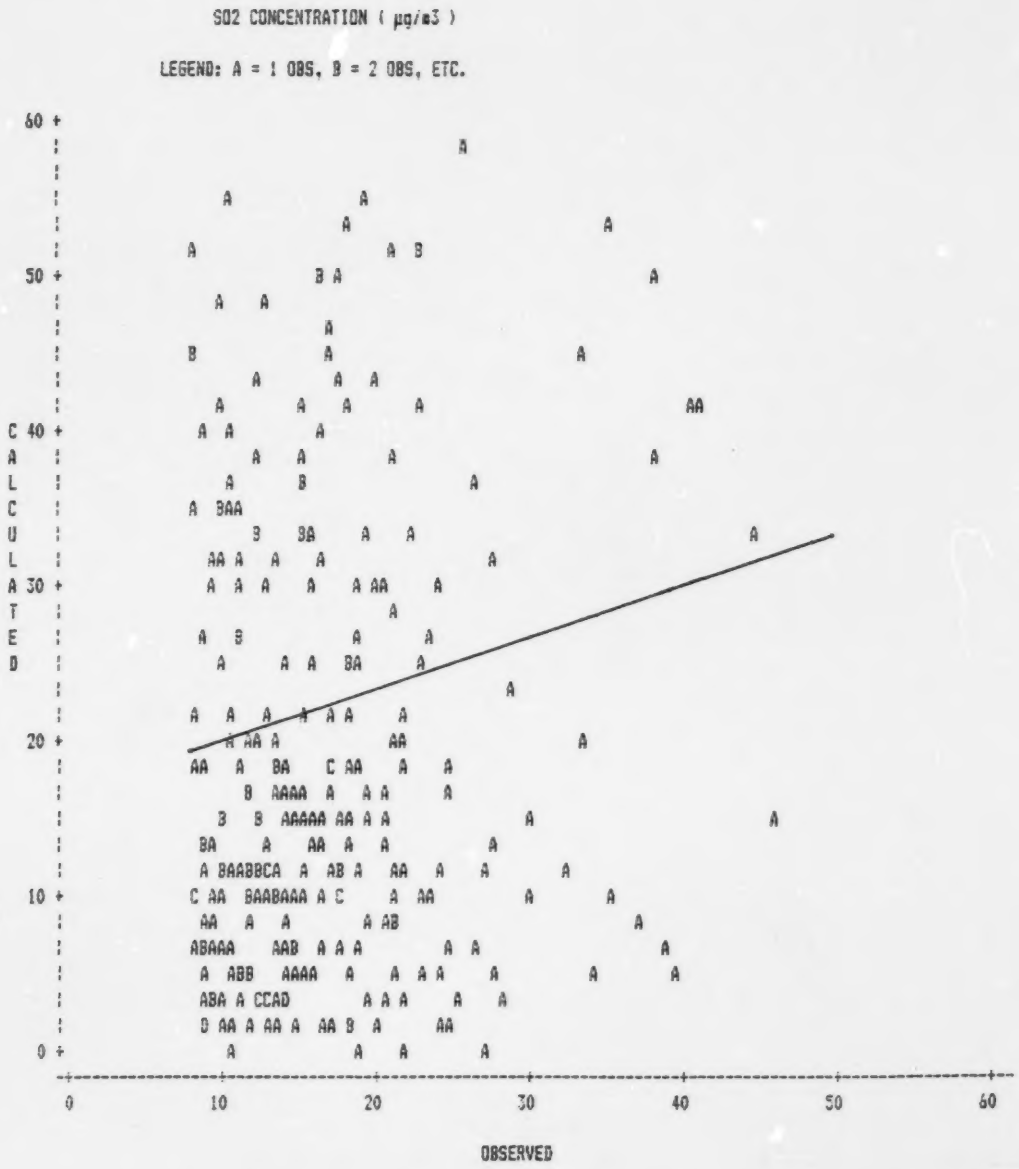


Figure 20. Comparison of calculated and observed 12-hour average $SO_2$ concentrations for the evaluation period.

TABLE 3

Summary of PEM-2 Evaluation Statistics for $SO_2$.

| | Total | | Day | | Night | |
|---|---|---|---|---|---|---|
| | Obs. | Calc. | Obs. | Calc. | Obs. | Calc. |
| Observations | 289 | | 147 | | 142 | |
| Range | 8-46 | 0-150 | 8-46 | 0-91 | 8-39 | 0-150 |
| Mean | 16.77 | 22.48 | 17.02 | 16.03 | 16.52 | 29.15 |
| S.D. | 7.28 | 22.96 | 7.85 | 15.71 | 6.65 | 27.07 |
| R | 0.10 | | 0.18 | | 0.19 | |
| Slope | 0.33 | | 0.35 | | 0.37 | |
| Intercept | 17.00 | | 10.02 | | 23.12 | |
| Mean of $(P_i/O_i)$ | 1.51 | | 1.07 | | 1.96 | |
| S.D. of $(P_i/O_i)$ | 1.66 | | 1.46 | | 1.98 | |
| Bias | -5.71 | | 0.99 | | -12.63 | |
| S.D. of Difference | 23.36 | | 16.28 | | 27.29 | |
| Average Absolute Gross Error | 15.42 | | 11.45 | | 19.53 | |
| RMSE | 24.00 | | 16.25 | | 29.99 | |
| Index of Agreement | 0.27 | | 0.43 | | 0.21 | |
| Mean Fractional Error | -0.46 | | 0.75 | | -1.71 | |
| MSE(u) | 519.67 | | 237.55 | | 721.90 | |
| MSE(s) | 56.48 | | 26.53 | | 177.31 | |
| MSE(u)/MSE | 90% | | 81% | | 80% | |
| MSE(s)/MSE | 10% | | 19% | | 20% | |

Note: The units of Range, Mean, S.D., Intercept, Bias, S.D. of Difference, Average Absolute Gross Error, and RMSE are $\mu g/m^3$.

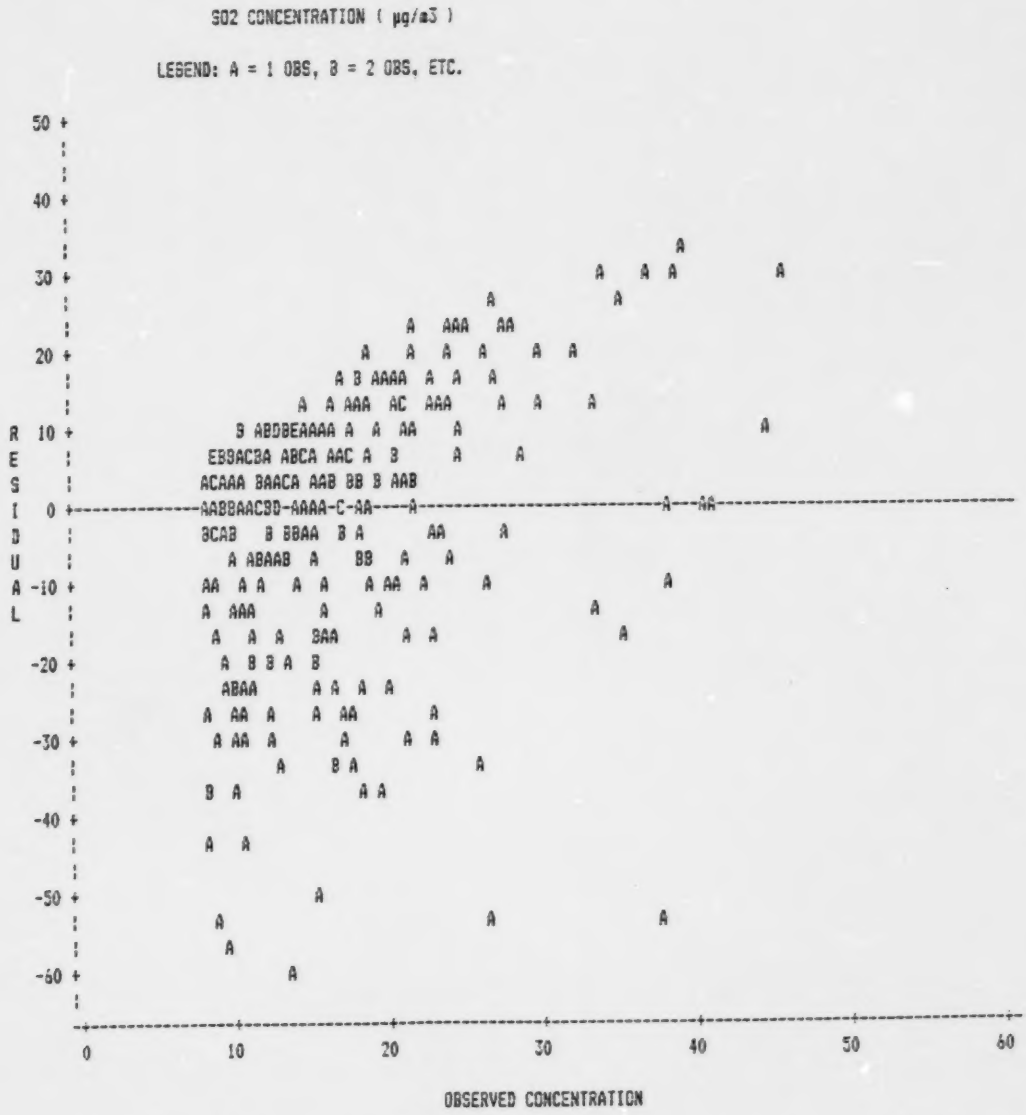


Figure 21. $SO_2$ residuals ($D_i = O_i - P_i$) versus observed 12-hour average $SO_2$ concentrations for the evaluation period.

the surface area source emissions; on the other hand, point sources contribute significantly during the daytime. If more of the emissions were treated as point sources, the result would be to increase the daytime concentrations, and decrease the concentrations at night. Thus, the model results are sensitive to the characterization of emissions. Ruff (1983), and Turner and Irwin (1985), identified the inclusion of point sources in the RAPS emissions inventory as area sources as a possible cause of the stability bias in the urban model (RAM) performance, whereby the largest concentrations are often predicted to occur with stable conditions and low wind speeds, in contrast to the observations.

Figure 22 shows a comparison of the calculated and observed daily (24 hour average) concentrations of $SO_2$ (averaged over all six stations for each of the 29 evaluation days). In general, the calculated daily concentrations are within a factor of two of the corresponding observed values, except for days 2, 18, and 23. If we plot the daytime and nighttime 12-hour average data separately (Figs. 23 and 24), we find that the large differences between the calculated and observed concentrations occured mostly during the night. These results confirm that the model performs much better during the day than at night, as noted above. Even at night, however, the major part of the error (about 80 percent) for $SO_2$ is unsystematic. This means that, for the given data set, PEM-2 is predicting with a high degree of accuracy, and we cannot readily identify where further improvements can be made to the model.

In order to test whether the optional new plume rise equations and plume penetration schemes of PEM-2 used in this evaluation made any difference, the model is rerun with the standard plume rise equations and the standard "all or none" penetration criterion to calculate the hourly

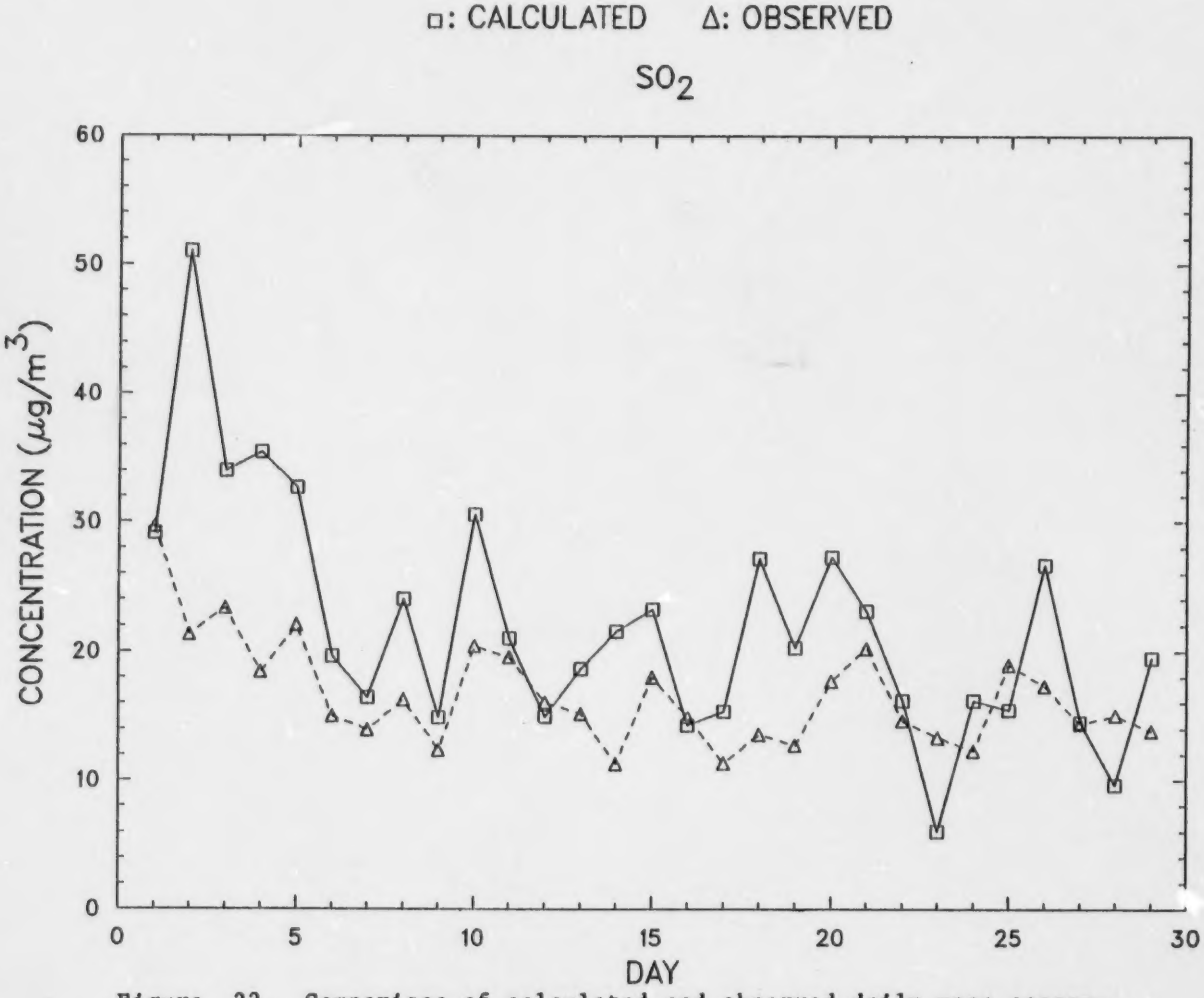


Figure 22. Comparison of calculated and observed daily mean concentrations of $SO_2$ (averaged over all PAFS stations) for the evaluation period.

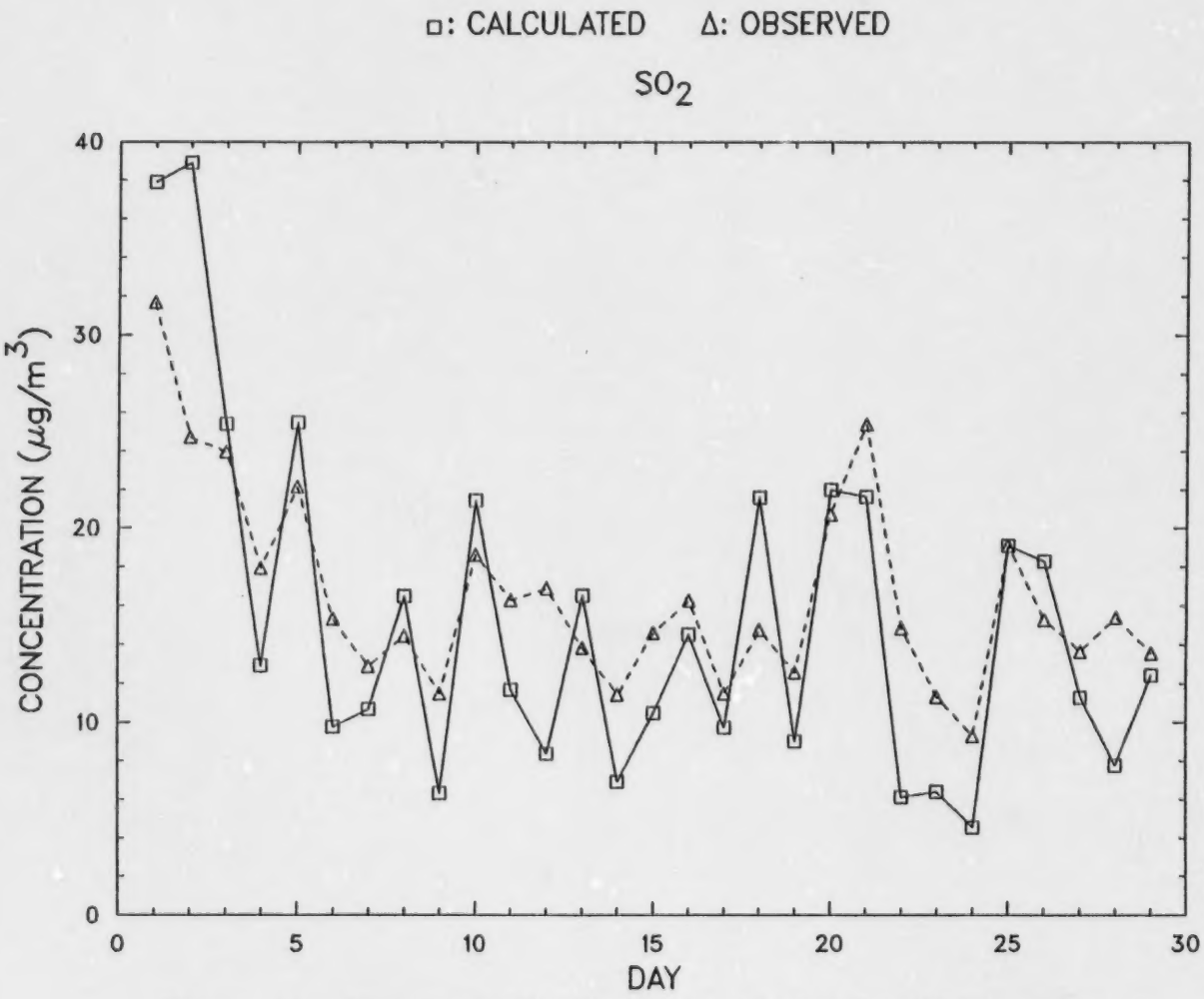


Figure 23. Same as in Fig. 22, except for daytime (12-hour average) $SO_2$ concentrations.

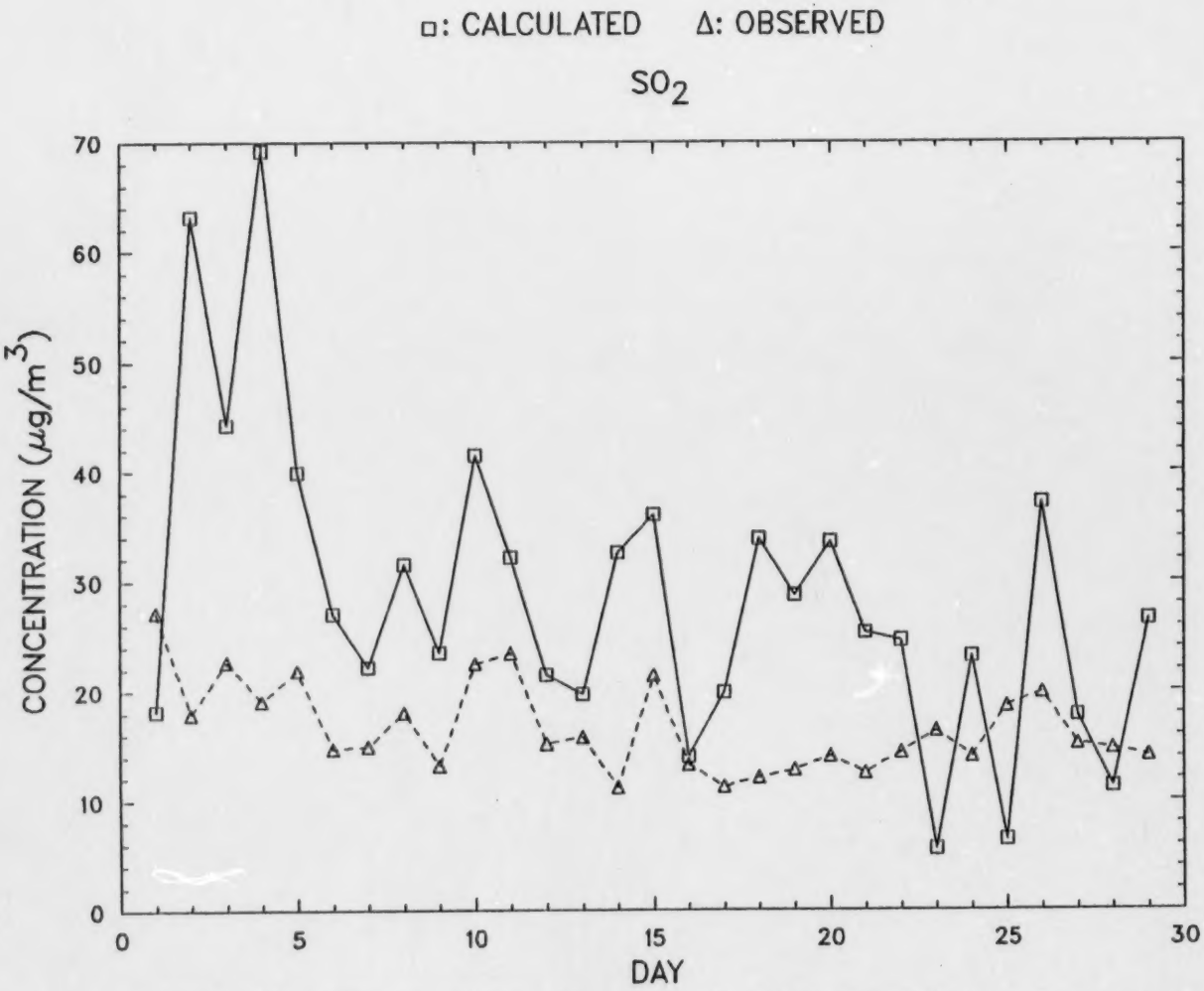


Figure 24. Same as in Fig. 22, except for nighttime (12-hour average) $SO_2$ concentrations.

$SO_2$ GLC for two days. Except for transition periods with sharp changes in stability and mixing height, no significant differences are noticeable in the calculated values. This is probably due to the fact that area sources are significant contributors to the $SO_2$ GLC in Philadelphia. Furthermore, the stack heights of point sources in the inventory are fairly low (under 100 m) and the plumes are not very buoyant. These plume conditions together with the high mixing depths input to the model did not give complete penetration. This limited testing of the the new plume rise and penetration schemes in this evaluation, therefore, did not permit a conclusive assessment of these methods. We would need a more suitable and better-defined data set for this purpose.

## SULFATE

The scatterplot of calculated versus observed 12-hour average fine sulfate concentrations is shown in Fig. 25. The linear regression fit is also shown in the figure. The statistics for this evaluation are given in Table 4.

The mean of ratios of calculated and observed values, $P_i/O_i$, is 1.45; the correlation coefficient is 0.77 and the slope is 0.84 both day and night. Since the background is estimated to be a large (25% or more) part the observed GLC, this high correlation suggests that the background concentrations, arising from long-range transport and regional inflow of the species across model boundaries, may be decisive in determining the particulate sulfate levels in urban areas. The high value of 0.87 for the index of agreement both day and night suggests that the background

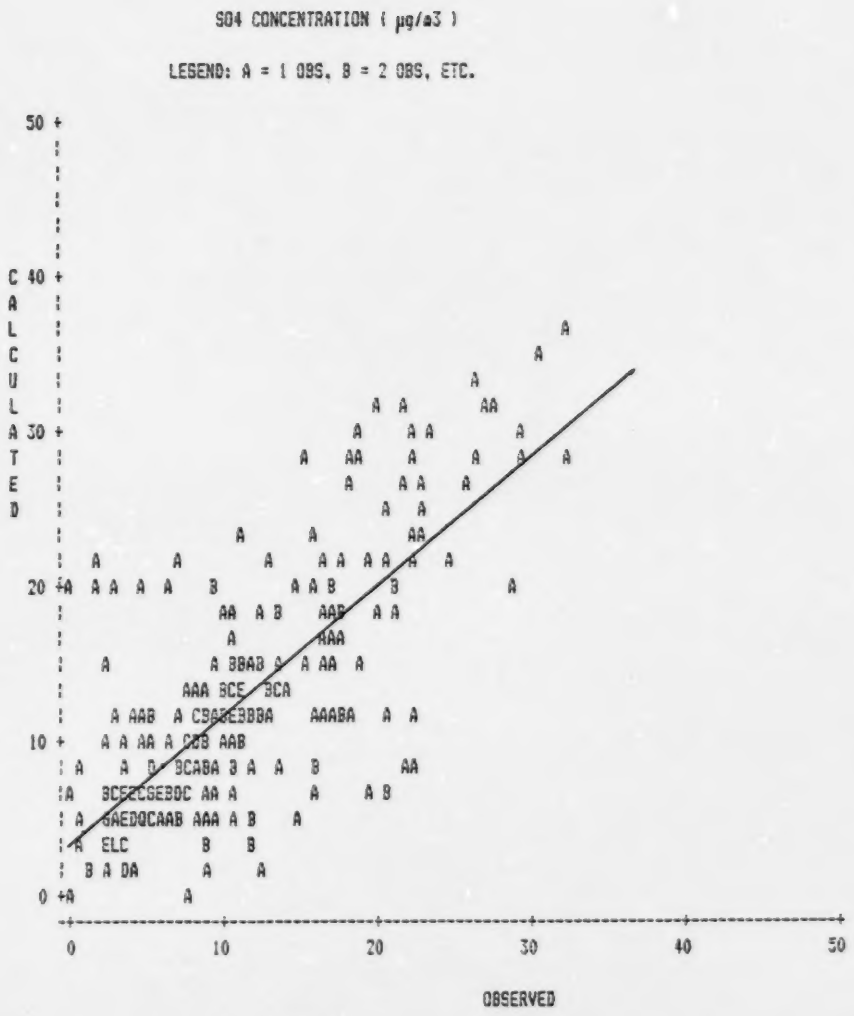


Figure 25. Comparison of calculated and observed 12-hour average sulfate concentrations for the evaluation period.

TABLE 4

Summary of PEM-2 Evaluation Statistics for Sulfate.

| | Total | | Day | | Night | |
|---|---|---|---|---|---|---|
| | Obs. | Calc. | Obs. | Calc. | Obs. | Calc. |
| Observations | 307 | | 152 | | 155 | |
| Range | 0-33 | 0-36 | 0-29 | 1-32 | 0-33 | 0-36 |
| Mean | 9.85 | 11.17 | 9.19 | 10.18 | 10.51 | 12.13 |
| S.D. | 6.91 | 7.54 | 6.04 | 6.58 | 7.63 | 8.24 |
| R | 0.77 | | 0.77 | | 0.77 | |
| Slope | 0.84 | | 0.84 | | 0.84 | |
| Intercept | 2.87 | | 2.48 | | 3.36 | |
| Mean of $(P_i/O_i)$ | 1.45 | | 1.46 | | 1.44 | |
| S.D. of $(P_i/O_i)$ | 1.89 | | 2.37 | | 1.25 | |
| Bias | -1.31 | | -1.00 | | -1.62 | |
| S.D. of Difference | 4.91 | | 4.32 | | 5.43 | |
| Average Absolute Gross Error | 3.42 | | 2.86 | | 3.97 | |
| RMSE | 5.08 | | 4.42 | | 5.65 | |
| Index of Agreement | 0.87 | | 0.87 | | 0.87 | |
| Mean Fractional Error | -0.42 | | -0.31 | | -0.52 | |
| MSE(u) | 22.87 | | 17.61 | | 27.67 | |
| MSE(s) | 2.91 | | 1.94 | | 4.21 | |
| MSE(u)/MSE | 89% | | 90% | | 87% | |
| MSE(s)/MSE | 11% | | 10% | | 13% | |

Note: The units of Range, Mean, S.D., Intercept, Bias, S.D. of Difference, Average Absolute Gross Error, and RMSE are $\mu g/m^3$.

concentrations determined as described earlier may be appropriate.

The sulfate residuals are plotted against the observed concentrations in Fig. 26. No clear bias in predictions is evident in the results. The mean difference over the entire range of concentrations is -1.31 $\mu g/m^3$, i.e., the model slightly overpredicts the sulfate GLC. The RMSE is 5.08 $\mu g/m^3$, and about 89 percent of the MSE is unsystematic. This suggests that PEM-2 performs well in simulating the PAFS sulfate concentrations resulting from the background contributions and primary emissions of the species, and chemical transformation of $SO_2$.

In order to investigate the role of background concentrations in the correlation between the observed and calculated GLC, a stepwise regression analysis has been performed. This consists of fitting regression relations between the observed GLC values as dependent variables, and the background and model-calculated concentrations as independent variables in a stepwise procedure, as follows:

Step 0 : $Y = a_1 + e_1$

Step 1 : $Y = a_2 + b_2 X + e_2$

Step 2 : $Y = a_3 + b_3 X + c_3 Z + e_3$

where $Y = O_i$ , the observed ground-level concentrations,

$X = B_i$ , the estimated background concentrations,

$Z = P_i - B_i$ , the model-calculated concentrations,

$e_k$ = the residual errors, (k = 1, 2, 3),

and $a_k$ , $b_k$ , and $c_k$ are the regression coefficients. At each step, the residual error, e, and correlation coefficient, R, are calculated to see if a reduction in the sum of squared errors (SSE) and an increase in the

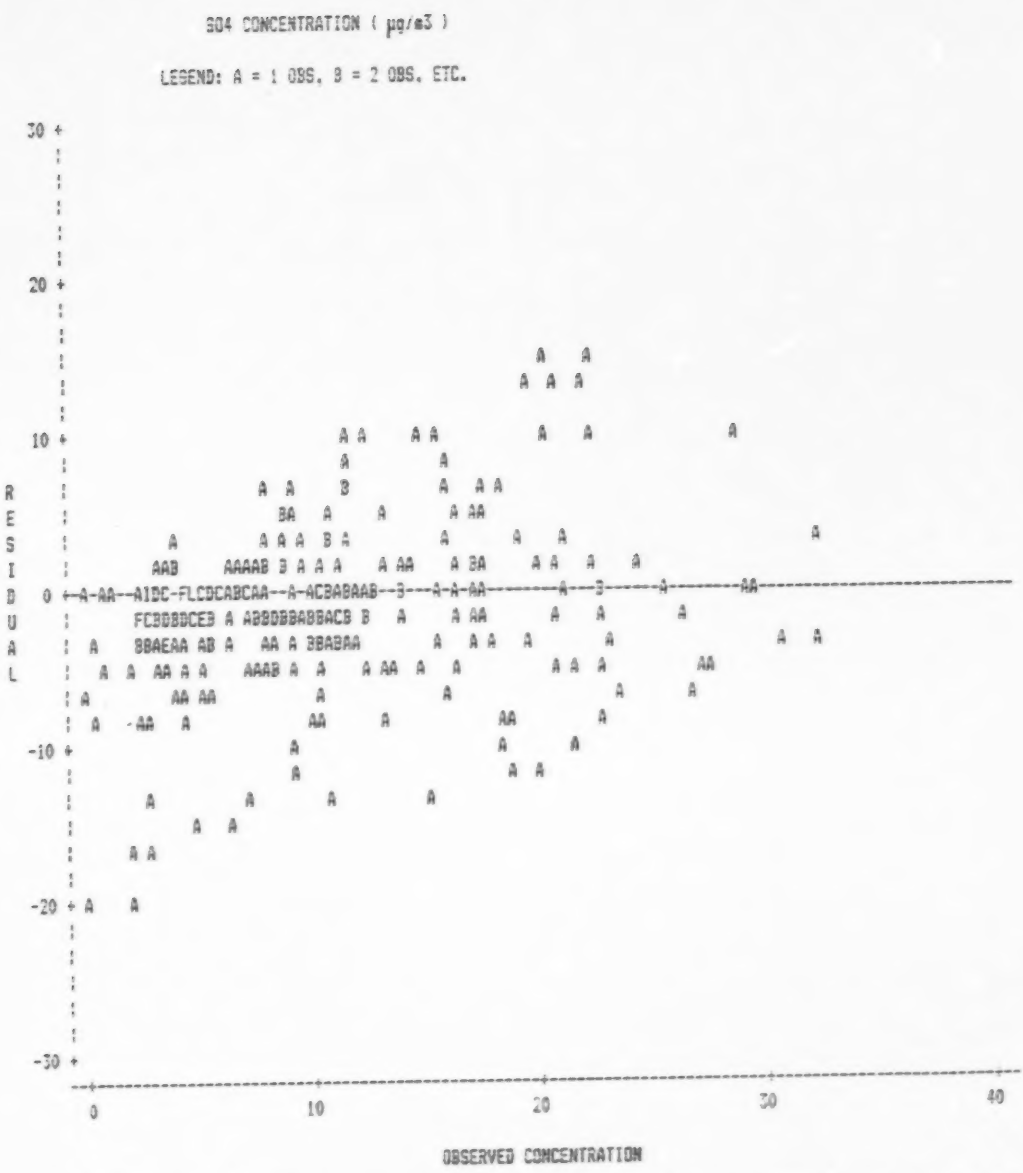


Figure 26. Sulfate residuals ($D_i = O_i - P_i$) versus observed sulfate concentrations for the evaluation period.

square of correlation coefficient (RSQ) occurs with the increase in the number of independent variables in the regression.

The stepwise regression equations, and the corresponding values of RSQ and SSE, are determined separately for the total, daytime, and nighttime observed sulfate GLC data, as shown in Table 5. The coefficients for the model-calculated concentrations in the regression equations are smaller than those for the background concentrations. This indicates that the latter account for a larger fraction of the correlation between the observed and predicted GLC than the local source contributions calculated by the model. This is particularly noticeable at nighttime, thus suggesting that either a major portion of the observed concentrations is due to the background, or that the model is not geared towards estimating the GLC at night. The decrease in SSE from step 0 to step 1 is much larger than that from step 1 to step 2 in all cases, especially at night. This confirms that background concentrations play a more important role at night for sulfate.

Figure 27 shows a comparison of the calculated and observed daily mean concentrations of sulfate (averaged over all six PAFS stations) for each of the 29 evaluation days. There is excellent agreement between the calculated and observed concentrations. If the results are plotted separately for 12-hour averages, the differences in model performance between daytime and nighttime (Figs. 28 and 29) are seen to be small.

TABLE 6

Results of Stepwise Regression Analysis for Sulfate.

| | RSQ | SSE |
|---|---|---|
| Total Data (sample size = 307) | | |
| Step 0 : Y = 9.85 , | - | 14608 |
| Step 1 : Y = 2.98 + 0.83 X , | 0.59 | 6056 |
| Step 2 : Y = 2.08 + 0.80 X + 0.40 Z , | 0.62 | 5585 |
| Daytime Data (sample size = 152) | | |
| Step 0 : Y = 9.19 , | - | 5506 |
| Step 1 : Y = 3.15 + 0.75 X , | 0.51 | 2703 |
| Step 2 : Y = 2.00 + 0.73 X + 0.60 Z , | 0.59 | 2236 |
| Nighttime Data (sample size = 155) | | |
| Step 0 : Y = 10.51 , | - | 8968 |
| Step 1 : Y = 3.02 + 0.88 X , | 0.64 | 3249 |
| Step 2 : Y = 2.52 + 0.86 X + 0.19 Z , | 0.64 | 3199 |

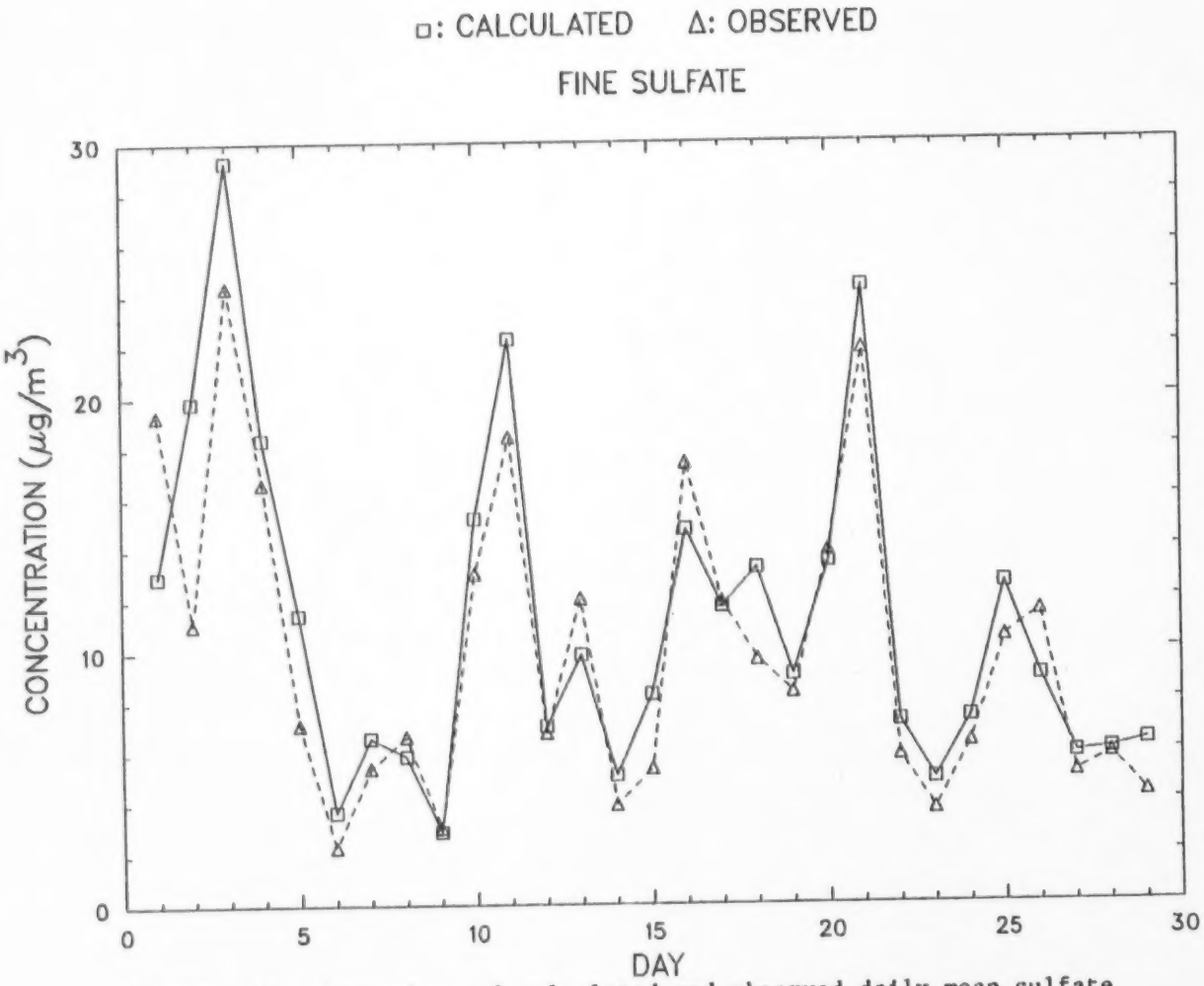


Figure 27. Comparison of calculated and observed daily mean sulfate concentrations (averaged over all PAFS stations) for the evaluation period.

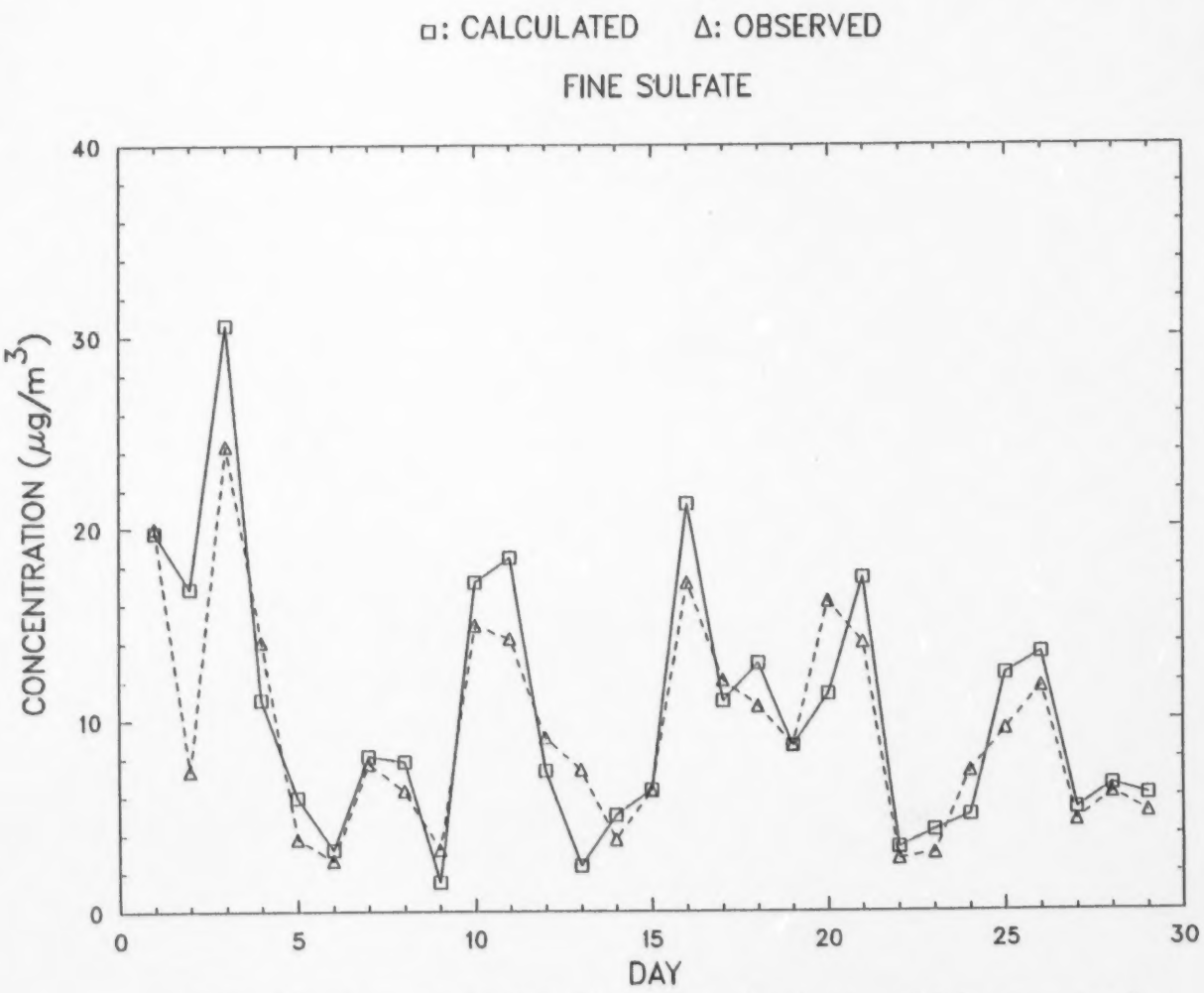


Figure 28. Same as in Fig. 27, except for daytime (12-hour average) sulfate concentrations.

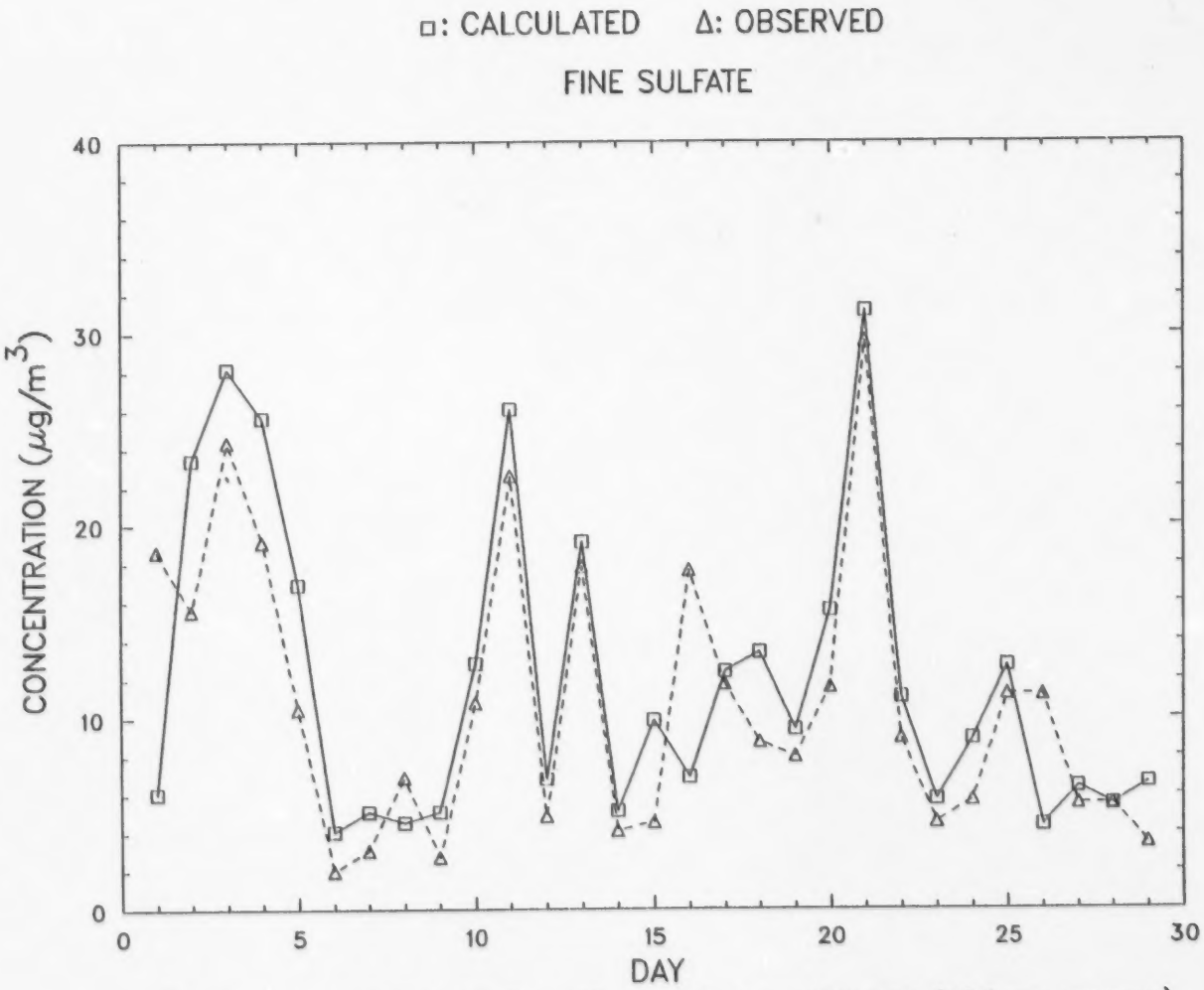


Figure 29. Same as in Fig. 27, except for nighttime (12-hour average) sulfate concentrations.

FINE TOTAL MASS

Figure 30 shows a comparison of all of the calculated and observed 12-hour average fine total mass concentrations for the model evaluation days. The solid line shows the linear regression fit with a slope of 0.79 and intercept of 10.91 $\mu g/m^3$.

The evaluation statistics of paired comparisons for fine total mass are summarized in Table 6. The high values of the correlation coefficient (0.75) and the index of agreement (0.84) indicate that the model performs well in predicting observed concentrations. However, the invariance of these values both day and night suggest that the background concentrations may be more important than local source contributions in estimating the FP concentrations in Philadelphia.

The fine total mass residuals are plotted against the observed concentrations in Fig. 31. A tendency towards overprediction is evident in the plot. The bias over the entire range of comparison is -4.7 $\mu g/m^3$. The nighttime bias (-5.39 $\mu g/m^3$) is higher than that during the daytime (-4.01 $\mu g/m^3$). The RMSE is 9.98 $ug/m^3$, and the major part (71 percent) of the MSE is unsystematic error. This suggests that PEM-2 performed satisfactorily in simulating the 12-hour average GLC of FP total mass in the PAFS data. In order to investigate the importance of FP background concentrations in Philadelphia, a stepwise regression analysis (similar to that described for sulfate) has been performed. The regression equations, RSQ, and SSE for each step are shown in Table 7. These results show that the FP background concentrations play a major role in correlating to the observed GLC, and the model-calculated concentrations are only of secondary importance.

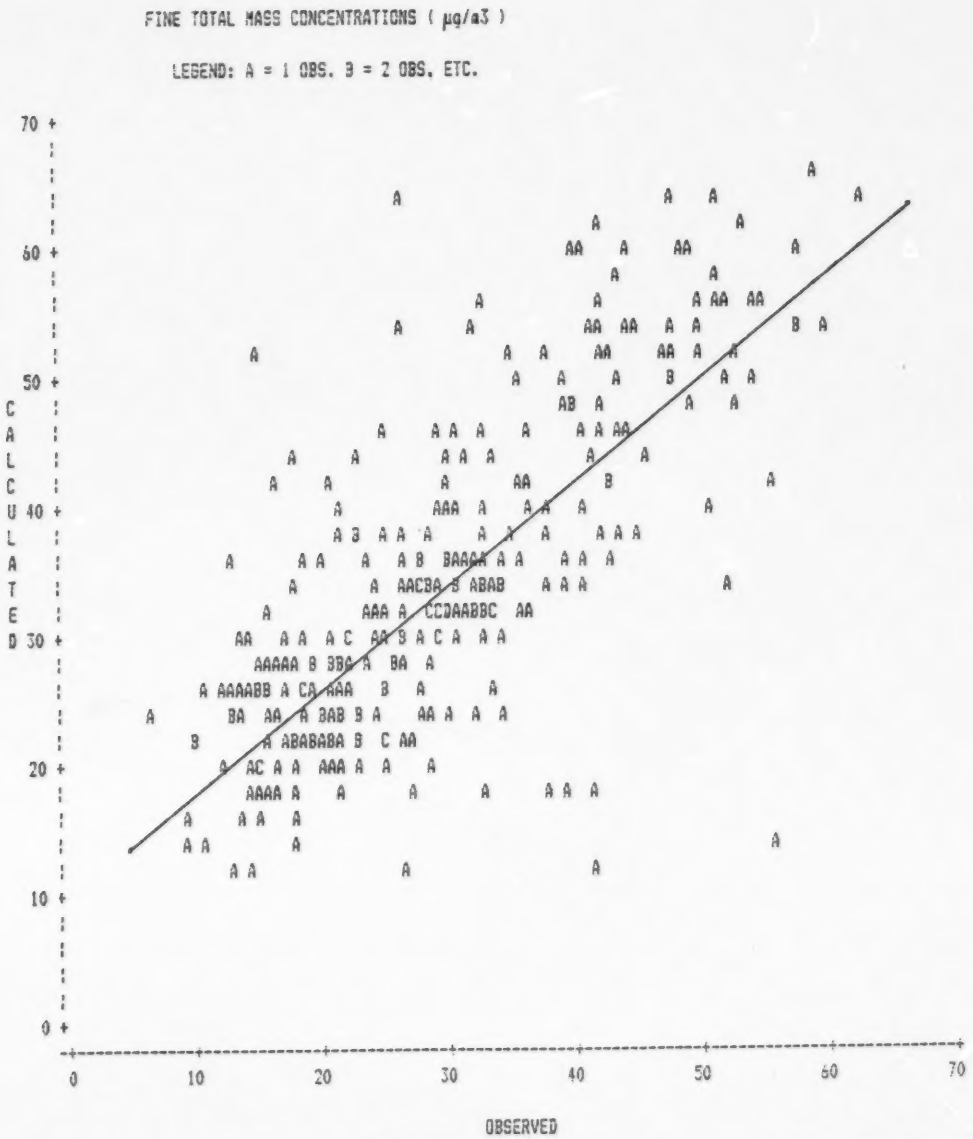


Figure 30. Comparison of calculated and observed 12-hour average FP total mass concentrations for the evaluation period.

TABLE 6

Summary of PEM-2 Evaluation Statistics for Fine Total Mass.

| | Total | | Day | | Night | |
|---|---|---|---|---|---|---|
| | Obs. | Calc. | Obs. | Calc. | Obs. | Calc. |
| Observations | 301 | | 150 | | 151 | |
| Range | 7-65 | 11-76 | 9-59 | 11-66 | 7-65 | 11-76 |
| Mean | 29.84 | 34.54 | 29.34 | 33.35 | 30.33 | 35.72 |
| S.D. | 12.15 | 12.81 | 11.34 | 11.83 | 12.93 | 13.65 |
| R | 0.75 | | 0.75 | | 0.75 | |
| Slope | 0.79 | | 0.78 | | 0.80 | |
| Intercept | 10.91 | | 10.46 | | 11.56 | |
| Mean of $(P_i/O_i)$ | 1.24 | | 1.20 | | 1.27 | |
| S.D. of $(P_i/O_i)$ | 0.41 | | 0.37 | | 0.45 | |
| Bias | -4.70 | | -4.01 | | -5.39 | |
| S.D. of Difference | 8.82 | | 8.24 | | 9.33 | |
| Average Absolute Gross Error | 7.43 | | 6.49 | | 8.37 | |
| RMSE | 9.98 | | 9.14 | | 10.75 | |
| Index of Agreement | 0.84 | | 0.84 | | 0.83 | |
| Mean Fractional Error | -0.85 | | -0.74 | | -0.97 | |
| MSE(u) | 71.14 | | 61.28 | | 79.67 | |
| MSE(s) | 28.49 | | 22.27 | | 35.93 | |
| MSE(u)/MSE | 71% | | 73% | | 69% | |
| MSE(s)/MSE | 29% | | 27% | | 31% | |

Note: The unit of Range, Mean, S.D., Intercept, Bias, S.D. of Difference, Average Absolute Gross Error and RMSE are $\mu g/m^3$.

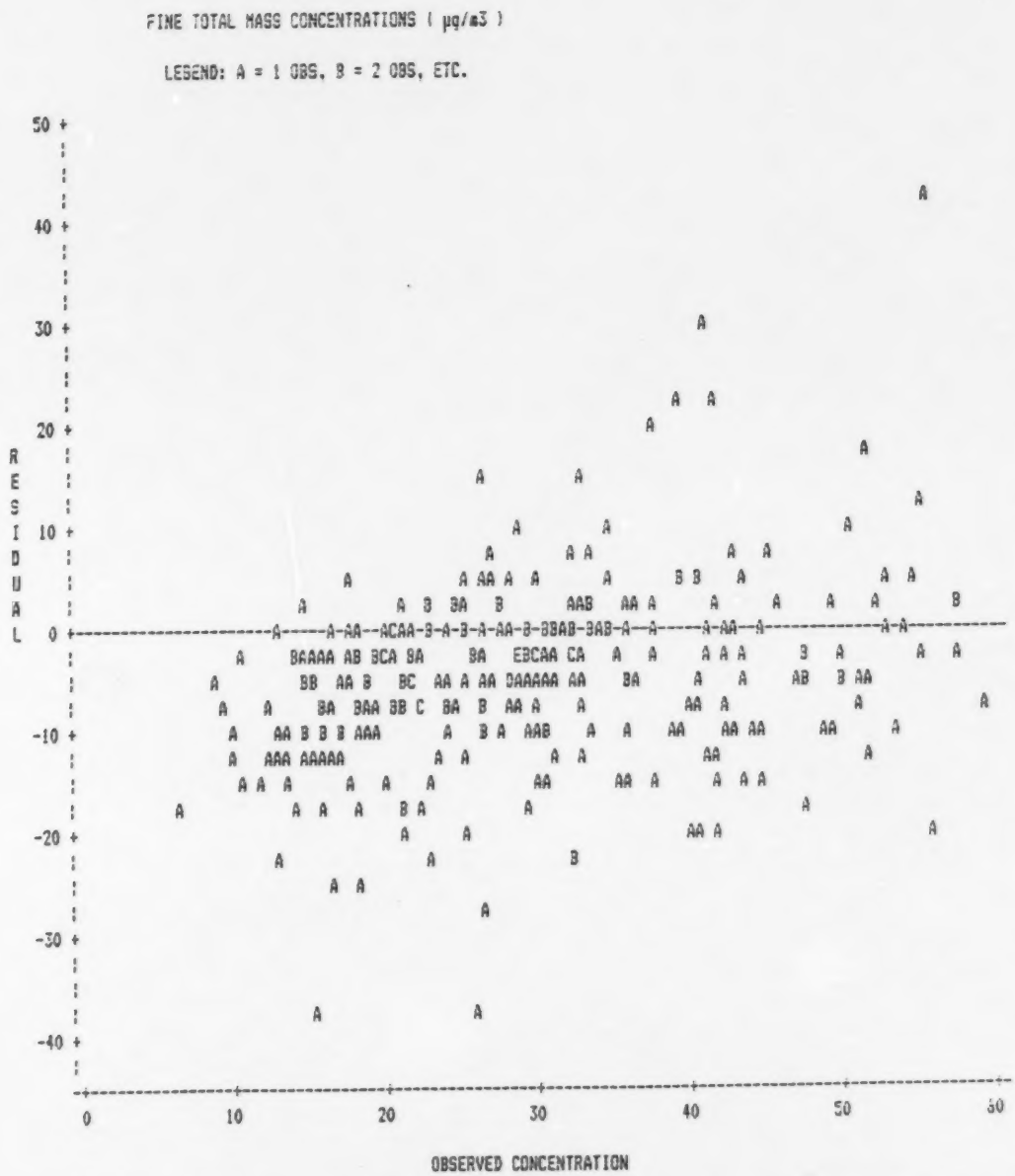


Figure 31. FP total mass residuals ($D_i = O_i - P_i$) versus observed 12-hour average FP concentrations for the evaluation period.

TABLE 7

Results of Stepwise Regression Analysis for Fine Total Mass.

| | RSQ | SSE |
|---|---|---|
| Total Data (sample size = 301) | | |
| Step 0 : Y = 29.84 , | - | 44316 |
| Step 1 : Y = 8.55 + 0.77 X , | 0.60 | 17634 |
| Step 2 : Y = 6.03 + 0.78 X + 0.36 Z , | 0.62 | 16895 |
| Daytime Data (sample size = 150) | | |
| Step 0 : Y = 29.34 , | - | 19158 |
| Step 1 : Y = 9.00 + 0.73 X , | 0.54 | 8771 |
| Step 2 : Y = 6.85 + 0.73 X + 0.39 Z , | 0.55 | 8539 |
| Nighttime Data (sample size = 151) | | |
| Step 0 : Y = 30.33 , | - | 25084 |
| Step 1 : Y = 8.30 + 0.81 X , | 0.66 | 8602 |
| Step 2 : Y = 5.69 + 0.81 X + 0.31 Z , | 0.67 | 8250 |

Figure 32 shows that the model tracks the observed daily mean concentrations (averaged over the six stations) fairly well for the evaluation period. Similar comparisons for the daytime and nighttime 12-hour average concentrations (Figs. 33 and 34, respectively) show no significant differences in performance.

COARSE TOTAL MASS

Figure 35 shows a comparison of the calculated and observed 12-hour average coarse total mass concentrations for the 29 evaluation days. The solid line shows the linear regression fit. The slope is 0.14 and the intercept is 13.45 $\mu g/m^3$.

The model evaluation statistics for coarse total mass are summarized in Table 8. The mean of ratios, $P_i/O_i$, is 1.29 and the corresponding standard deviation is 0.81. The correlation coefficient of 0.25 indicates a large degree of randomness in the paired comparison of coarse mass concentrations. The relatively low index of agreement (0.47) suggests that the predictions of CP contain more error than the results for FP and sulfate.

The coarse mass residuals are plotted against the observed concentrations in Fig. 36. The model shows a clear bias to overpredict the observed concentrations below 20 $\mu g/m^3$, and underpredict $O_i$ above this value. The mean of differences over the entire range of concentrations is -0.83 $\mu g/m^3$, i.e., the model is slightly conservative. The average absolute gross error of 5.74 $\mu g/m^3$ is much less than the mean of observed concentrations. The RMSE is 8.28 $\mu g/m^3$, but 73 percent of the MSE is systematic. This differs from the results for sulfate and FP for which a major part of the MSE is unsystematic. This seems to suggest that there is room for improvement in

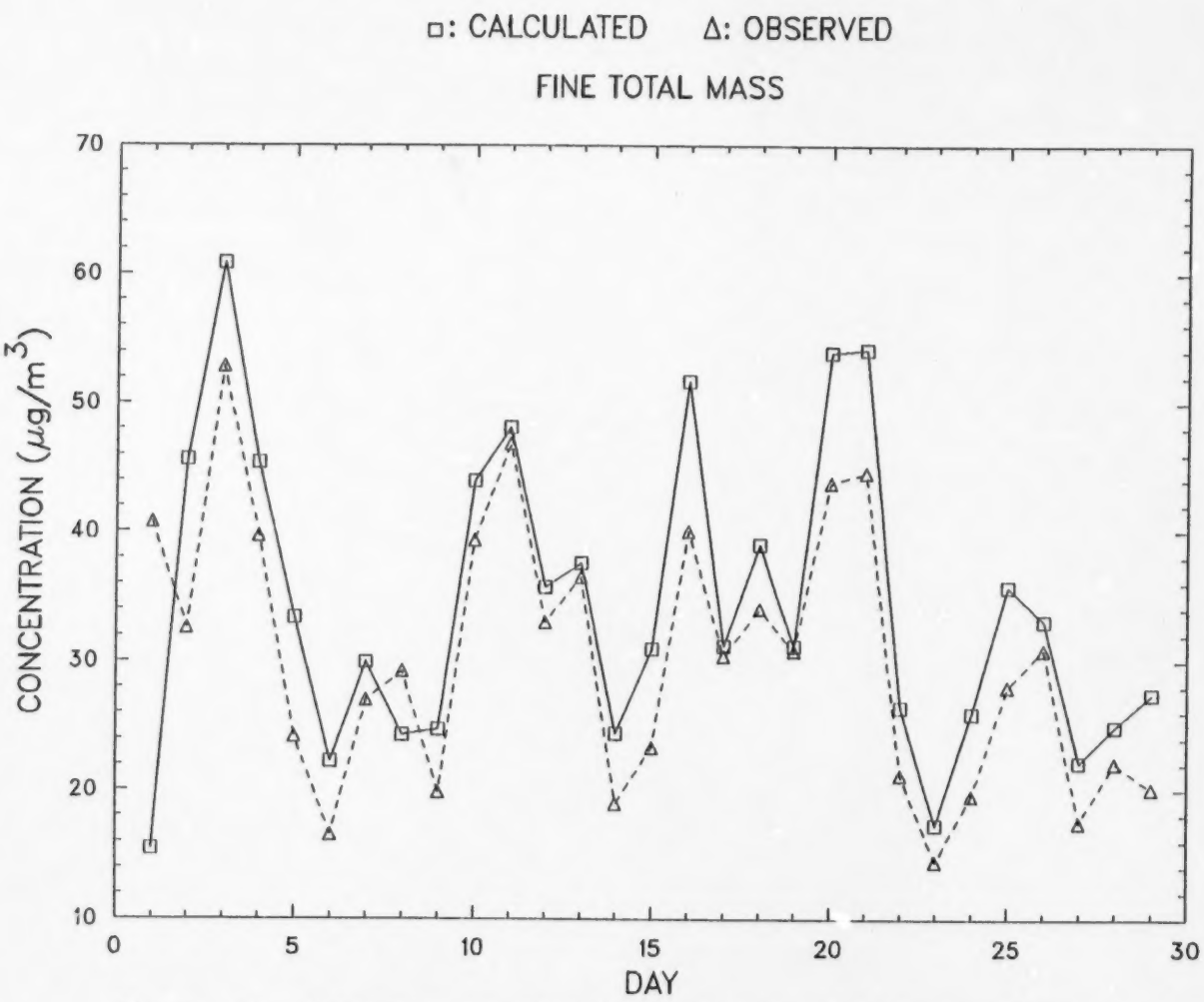


Figure 32. Comparison of calculated and observed daily mean FP total mass concentrations (averaged over all PAFS stations) for the evaluation period.

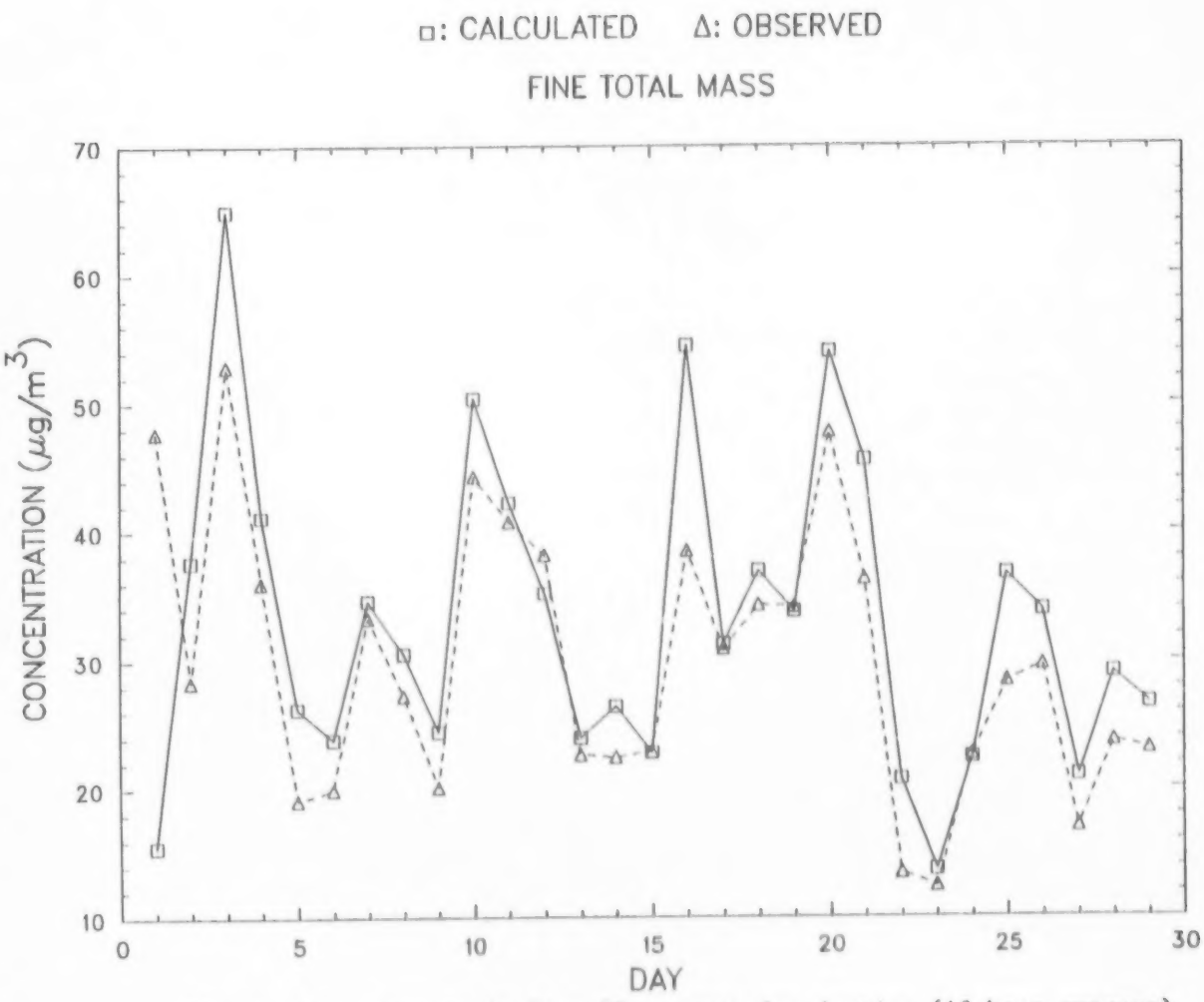


Figure 33. Same as in Fig. 32, except for daytime (12-hour average) FP total mass concentrations.

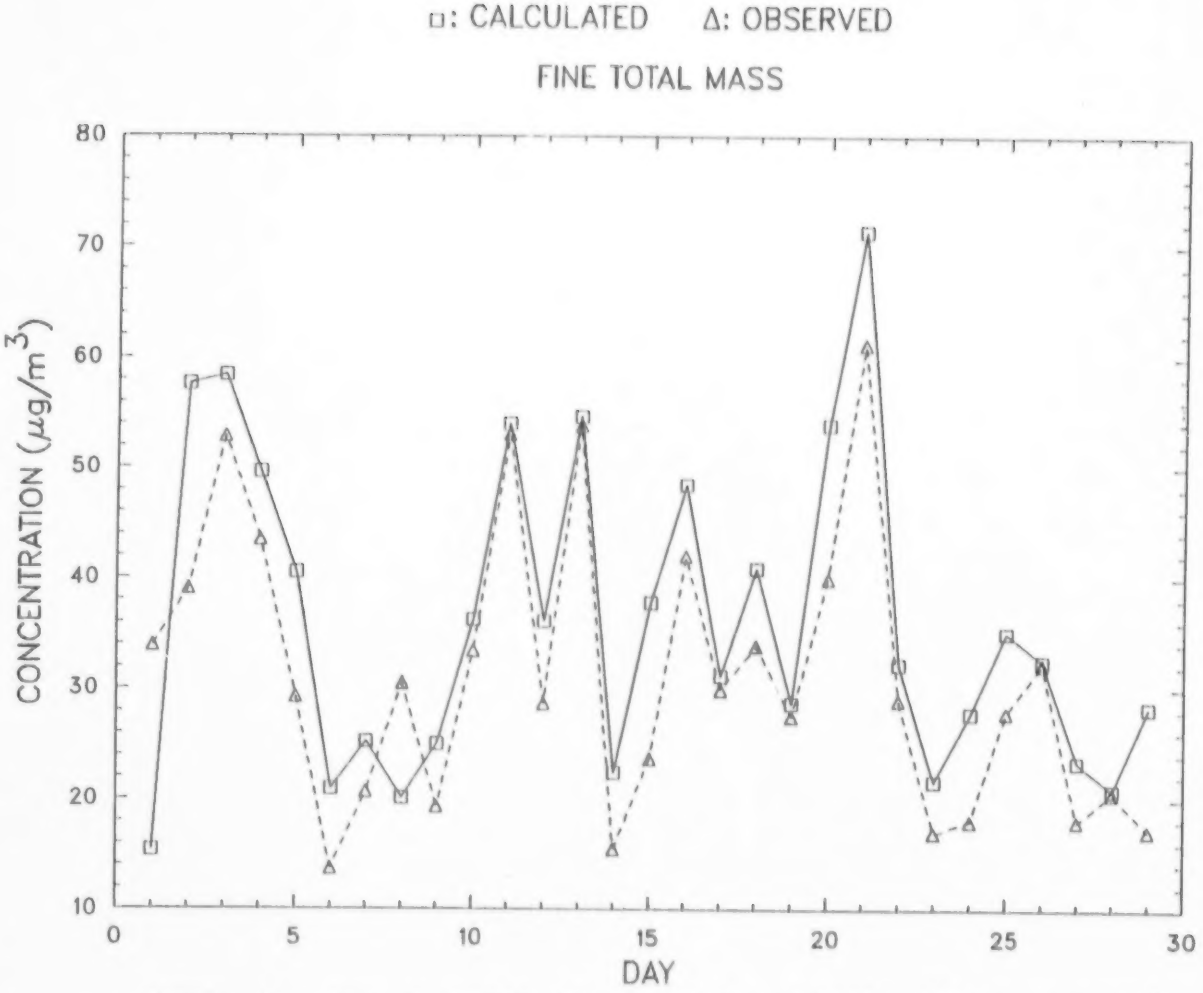


Figure 34. Same as in Fig. 32, except for nighttime (12-hour average) FP total mass concentrations.

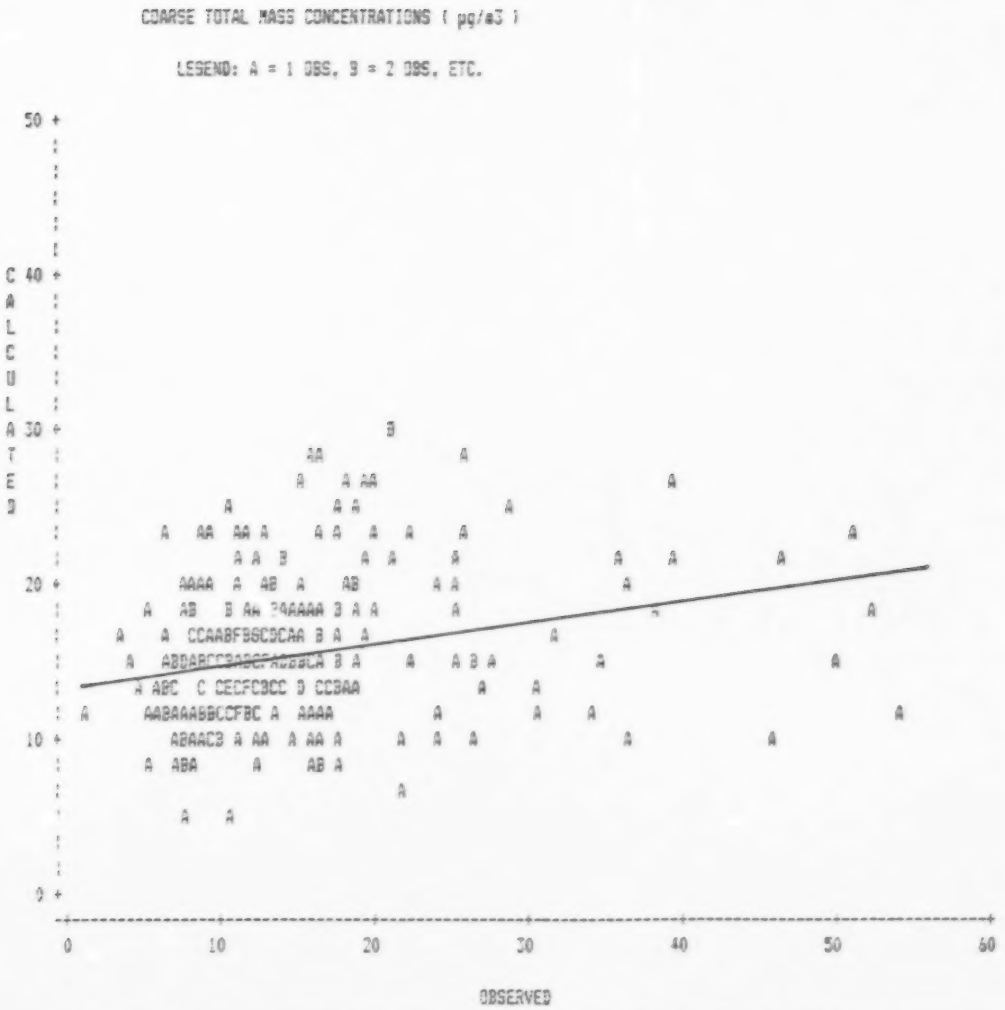


Figure 35. Comparison of calculated and observed 12-hour average CP total mass concentrations for the evaluation period.

TABLE 8

Summary of PEM-2 Evaluation Statistics for Coarse Total Mass.

| | Total | | Day | | Night | |
|---|---|---|---|---|---|---|
| | Obs. | Calc. | Obs. | Calc. | Obs. | Calc. |
| Observations | 298 | | 148 | | 150 | |
| Range | 1-54 | 5-31 | 1-47 | 7-26 | 3-54 | 5-31 |
| Mean | 14.62 | 15.44 | 13.39 | 14.89 | 15.84 | 16.00 |
| S.D. | 8.15 | 4.46 | 6.58 | 3.63 | 9.31 | 5.10 |
| R | 0.25 | | 0.25 | | 0.23 | |
| Slope | 0.14 | | 0.14 | | 0.13 | |
| Intercept | 13.45 | | 13.05 | | 14.01 | |
| Mean of $(P_i/O_i)$ | 1.29 | | 1.35 | | 1.22 | |
| S.D. of $(P_i/O_i)$ | 0.81 | | 0.98 | | 0.59 | |
| Bias | -0.83 | | -1.50 | | -0.16 | |
| S.D. of Difference | 8.25 | | 6.68 | | 9.53 | |
| Average Absolute Gross Error | 5.74 | | 4.90 | | 6.56 | |
| RMSE | 8.28 | | 6.82 | | 9.50 | |
| Index of Agreement | 0.47 | | 0.47 | | 0.45 | |
| Mean Fractional Error | -0.36 | | -0.52 | | -0.20 | |
| MSE(u) | 18.57 | | 12.27 | | 24.48 | |
| MSE(s) | 49.99 | | 34.26 | | 65.82 | |
| MSE(u)/MSE | 27% | | 26% | | 27% | |
| MSE(s)/MSE | 73% | | 74% | | 74% | |

Note: The unit of Range, Mean, S.D., Intercept, Bias, S.D. of Difference, Average Absolute Gross Error, and RMSE are $\mu g/m^3$.

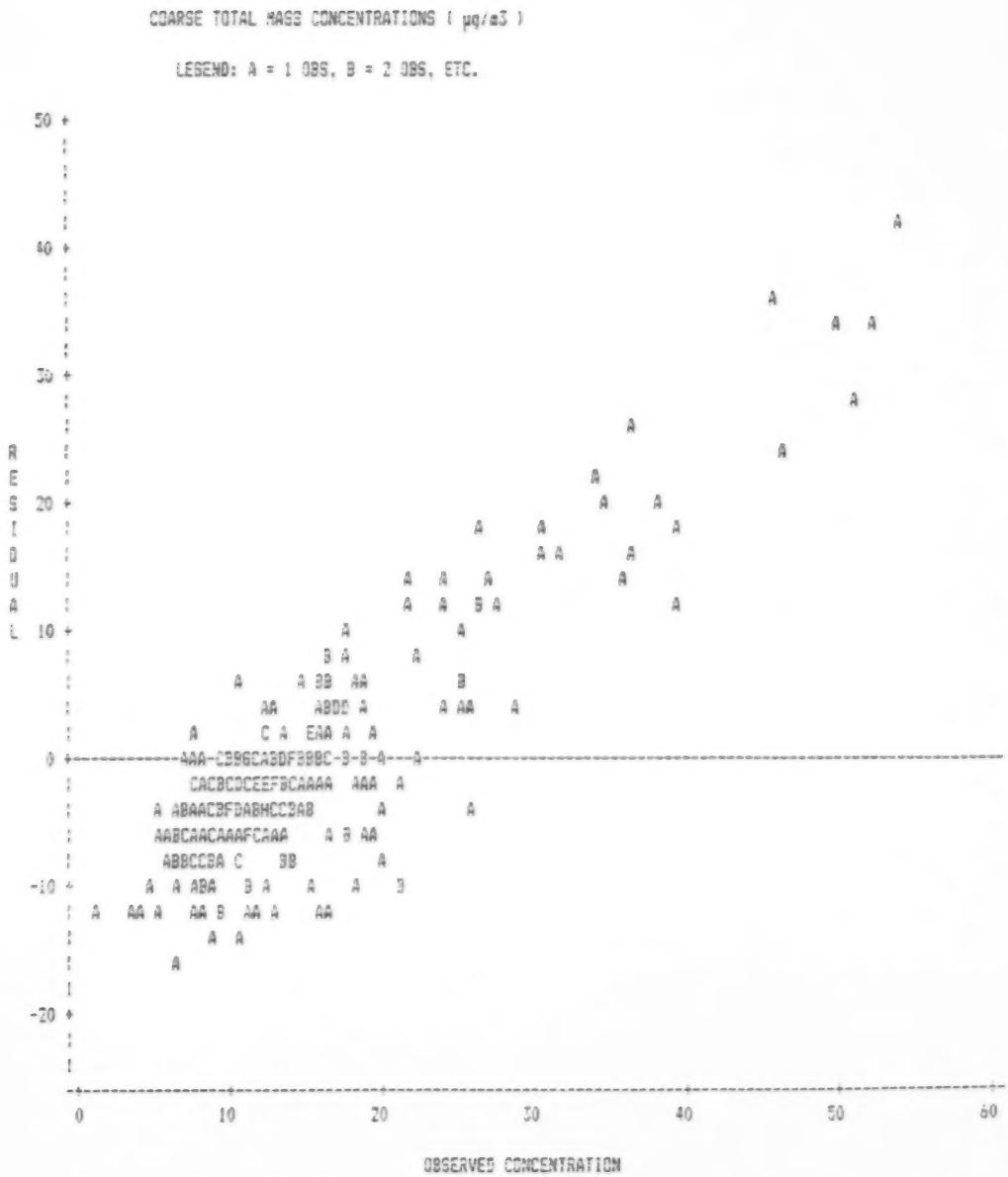


Figure 36. CP total mass residuals ($D_i = O_i - P_i$) versus observed 12-hour average CP concentrations over the evaluation period.

modeling the CP concentrations, for example, by using a different set of values for the deposition and gravitational settling velocities for particles of size 2.5 to 10 microns.

In order to investigate the role of background concentrations in the comparison between the observed and calculated GLC, a stepwise regression analysis has been performed for the total, daytime, and nighttime CP data separately. The regression equations, RSQ, and SSE for each step are shown in Table 9. The results show that the correlation coefficients for both background and model-calculated concentrations are of the same order, indicating that each accounts for about the same fraction of the correlation between the observed and predicted GLC. The decrease in SSE is more significant from step 0 to step 1 than from step 1 to step 2. However, this decrease is not so significant as that for the sulfate or FP species.

Figures 37, 38, and 39 show the model performance in predicting daily mean, daytime and nighttime (12-hour average) coarse total mass concentrations, respectively. All concentrations are averaged over the six PAFS stations. The overall agreement between the calculated and observed variations is good with no discernable difference between the daytime and nighttime performance. Though the local source contributions may be relatively more important for the coarse mass than for sulfate and fine mass, the background plays an important role in determining the overall CP concentration levels in Philadelphia.

TABLE 9

Results of Stepwise Regression Analysis for Coarse Total Mass.

| | | RSQ | SSE |
|---|---|---|---|
| Total Data (sample size = 298) | | | |
| Step 0 : | Y = 14.62 , | - | 19723 |
| Step 1 : | Y = 6.38 + 0.70 X, | 0.12 | 17264 |
| Step 2 : | Y = 3.84 + 0.72 X + 0.67 Z, | 0.16 | 16595 |
| Daytime Data (sample size = 148) | | | |
| Step 0 : | Y = 13.39, | - | 6364 |
| Step 1 : | Y = 6.25 + 0.61 X, | 0.11 | 5659 |
| Step 2 : | Y = 2.98 + 0.70x + 0.71 Z, | 0.15 | 5383 |
| Nighttime Data (sample size = 150) | | | |
| Step 0 : | Y = 15.84, | - | 12908 |
| Step 1 : | Y = 6.99 + 0.75 X, | 0.13 | 11166 |
| Step 2 : | Y = 5.23 + 0.73 X + 0.50 Z, | 0.15 | 10950 |

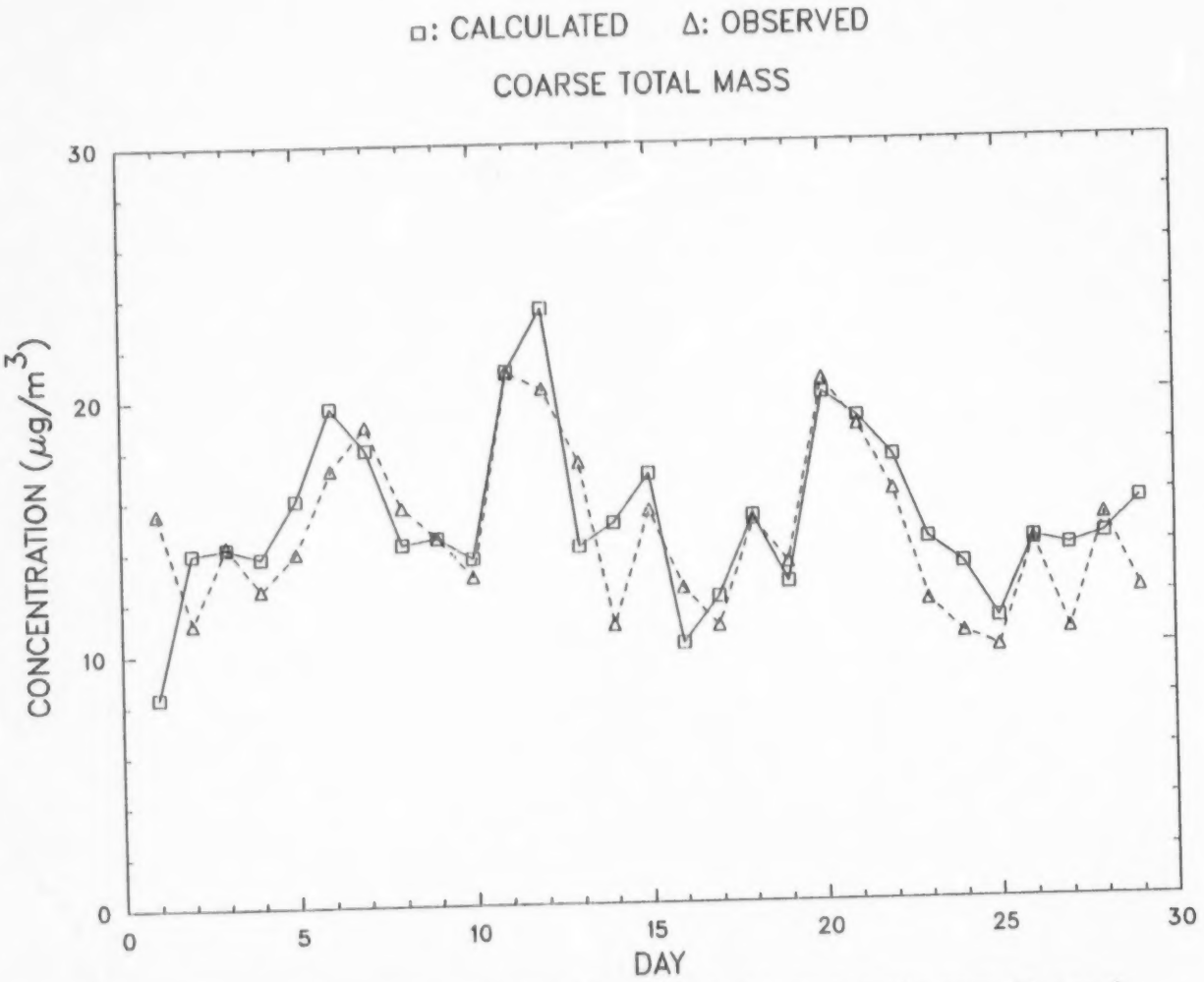


Figure 37. Comparison of calculated and observed daily mean CP total mass concentrations (averaged over all PAFS stations) for the evaluation period.

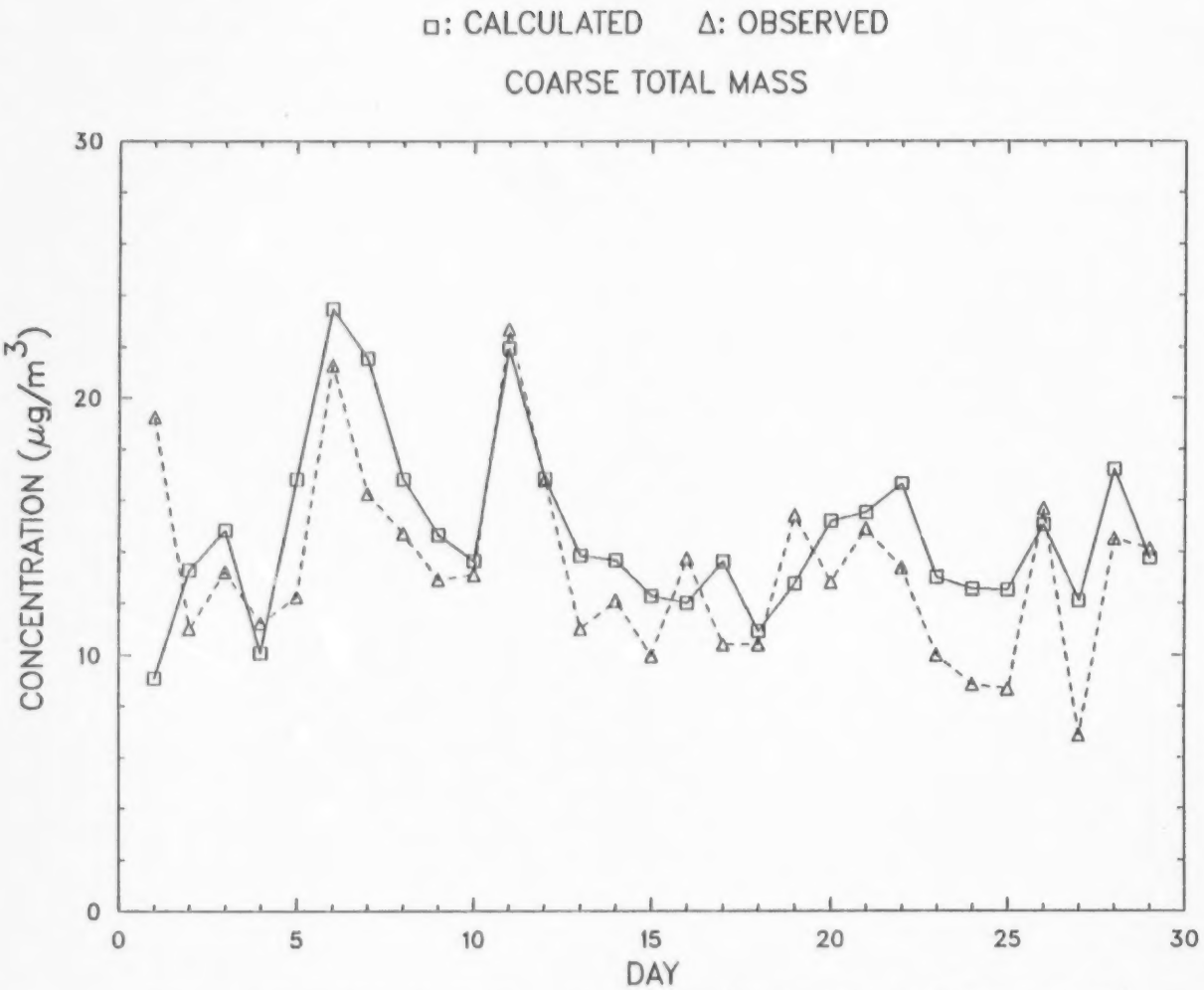


Figure 38. Same as in Fig. 37, except for daytime (12-hour average) CP total mass concentrations.

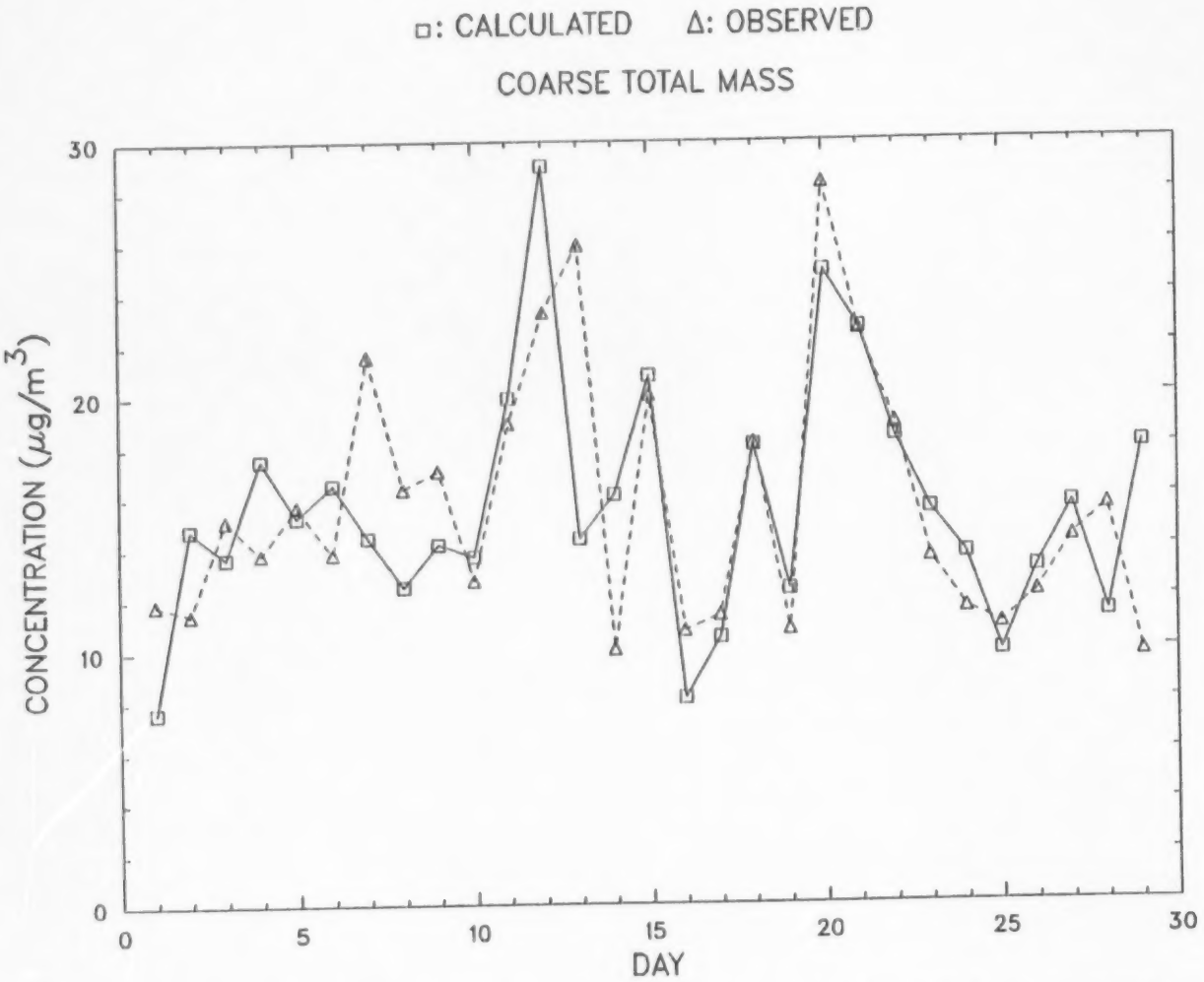


Figure 39. Same as in Fig. 37, except for nighttime (12-hour average) CP total mass concentrations.

# SECTION 5

# CONCLUSIONS

This report described an evaluation of the Pollution Episodic Model Version 2 using 29 days of the Philadelphia Aerosol Field Study data. This evaluation is designed to test the model performance by comparing its concentration estimates for four pollutant species ($SO_2$, sulfate, fine and coarse total mass) to the measured air quality data, using appropriate statistical measures of performance.

The emphasis in this evaluation is on primary fine and coarse inhalable urban particulate matter, as well as pollutants that undergo chemical transformation in the atmosphere to form fine secondary particulates (e.g., $SO_2$ to sulfate aerosol). For the evaluation period, PEM-2 predicted 12-hour average concentrations of $SO_2$, sulfate, fine and coarse total mass to within a factor of two, which is the best that may be expected considering the natural variability in model input data (Hanna, 1981).

The hourly $SO_2$ concentration data are considered to provide a demanding test of the performance of PEM-2, especially since the background $SO_2$ concentrations are assumed to be zero. The model performance for $SO_2$ is better during daytime than at nighttime, and generally better at the suburban stations, which are affected mostly by point sources, than at downtown stations. The latter are impacted heavily by the urban area sources, which are thought to be major contributors to the errors in the

concentration estimates. These errors result from the difficulty in characterizing area source emissions, lack of information on source conditions such as release height, plume rise, and building-wake effects, as well as the narrow plume concept and other simplifying assumptions used in the concentration algorithms for area sources.

The calculated and observed $SO_2$ concentrations are closer at all PAFS stations during daytime than at night. The model generally overestimates the hourly concentrations at night, and underpredicts during the day at rural locations which are not significantly impacted by area sources. This stability bias of the model is attributed to the the problems associated with modeling low-level urban sources, and the model sensitivity to the characterization and partition of emissions between point and area sources.

The model performance for the particulate species is good; both the 12-hour and daily mean concentrations (averaged over the six PAFS stations) over the evaluation period are predicted well. For sulfate and fine total mass, the values of the correlation coefficient and index of agreement are high, and a large part of the estimated MSE is unsystematic. For coarse total mass, the evaluation statistics are not as good by comparison, and the large systematic error suggests there is room for model improvement. On the average, the model estimates of concentrations for the particulate species are slightly conservative (overpredictions).

The overall good performance of the model for particulate species should be interpreted with caution since the background concentrations, resulting from long-range transport and regional inflow of species across model boundaries, far exceed the urban source contributions to the surface

concentrations in Philadelphia. When the wind direction changes significantly, no particular source contributes longer than one hour to receptor concentrations in PEM-2 (with the possible exception of receptors located within area sources). On the other hand, the determination of background concentrations from PAFS data is somewhat subjective due to the small number of monitoring stations available. Ideally, the background monitors should be located on the calculation grid boundaries, away from the influence of sources being modeled. Nevertheless, judging from the model performance in this evaluation, the values of background particulate concentrations estimated from observed GLC at suburban monitors and wind direction analysis for each 12-hour averaging period seem appropriate.

It appears that the background particulate concentrations are important not only in Philadelphia, but in other urban areas as well. Wolff et al. (1985) studied the influence of local and regional sources on the concentrations of inhalable particulate matter at four (urban, industrialized, suburban, and rural) sites in southeastern Michigan, and found that FP was dominated by regional influences rather than local influences at all four sites, while CP was dominated by local sources. The regional influences were most pronounced on the sulfate levels which accounted for the largest fraction (40 - 50%) of the FP in their study.

It may be possible to establish the relative importance of the local and regional contributions to the urban FP and CP concentrations from an analysis of the National Inhalable Particulate Network data. In a preliminary interpretation of these data, Pace and Rodes (1981) concluded that CP and FP concentration levels are substantially different among urban areas and, on an urban scale, FP averages are generally more homogeneous

indicating a regional pattern; the lower degree of uniformity in CP (compared to FP) concentrations in urban areas may be due to a larger contribution of CP from local sources. The results of the present study seem to support this conclusion.

The characteristics of emissions in Philadelphia appear to be substantially different from those in St. Louis. This is demonstrated in Table 10 which compares the daily average emission rates of the species from point and area sources during the PAFS and the RAPS experiments. Unlike in St. Louis, the area sources in Philadelphia are significant contributors of $SO_2$ and sulfate, and point source contributions to fine and coarse total mass are very important. Because of the differences in emission characteristics between different urban areas, it is desirable to evaluate PEM-2 with as many detailed data sets as possible. In an evaluation of PEM using St.Louis/RAPS data, Pendergrass and Rao (1984) attributed the large overpredictions of FP and CP by the model to overestimation of emission rates of area sources in the inventory and their incorrect location, among other factors.

The meteorological data used in this evaluation are surface observations from NWS station at the Philadelphia Airport (PHL). These data are only approximations to real conditions in the Philadelphia urban area. Errors in wind direction may cause the model to impact particular receptors which may be completely ignored in reality. Errors in wind speed and stability classification may significantly affect the diffusion, plume rise and penetration calculations. It is well known that the frequency and intensity of nocturnal inversions over cities are decreased due to enhanced thermal and mechanical mixing resulting from urban heat island and

TABLE 10

Comparison of Daily Average Emission Rates (kg/s) from Area and Point Sources in Philadelphia and St. Louis.

| Pollutant | Area Sources | Point Sources |
|---|---|---|
| | Philadelphia/PAFS | |
| $SO_2$ | 15.674 | 51.561 |
| Sulfate | 0.603 | 1.639 |
| Fine Total Mass | 5.459 | 3.997 |
| Coarse Total Mass | 3.400 | 1.637 |
| | St. Louis/RAPS | |
| $SO_2$ | 0.434 | 36.018 |
| Sulfate | 0.008 | 0.266 |
| Fine Total Mass | 2.518 | 0.211 |
| Coarse Total Mass | 6.631 | 0.921 |

increased roughness effects. Hence, the diffusion conditions in the lower atmosphere over cities tend to be of near-neutral type, without the strong diurnal variations (see Fig. 4) found at airport locations. The plume dispersion parameters used in PEM-2 account for the enhanced turbulence and mixing over urban areas by using greater sigma values (than in the open country) for given stability class. However, due to lack or unreliability of on-site meteorological data, it cannot be ascertained if the actual dispersion conditions over Philadelphia are adequately simulated in this study.

The effective height of area-source emissions, taken as 10 m (typical of building-top releases) in this evaluation, is an approximate value used to mitigate the large GLC calculated at receptors located within the area sources. Better characterization of area and point source emissions would be helpful. The influence of the new plume rise equations and new plume-penetration schemes used in this evaluation (for buoyancy-dominated point source plumes in unstable/neutral atmosphere) could not be assessed since no significant differences are noticeable in the hourly $SO_2$ GLC calculated for two days from the new schemes and the standard schemes, except for transition periods with sharp changes in stability and mixing height. However, these results are not conclusive, and more tests with suitable data are necessary to bring out the differences in performance between the various schemes.

The primary objective of this study is to evaluate the performance of PEM-2 with emphasis on estimating concentrations of urban particulate matter. Based on the results, we conclude that PEM-2 is able to simulate the observed concentrations of $SO_2$, sulfate, FP and CP total mass in PAFS

data fairly well. The results of stepwise regression analysis in this study suggest that the observed GLC of the urban particulate species are highly correlated to their estimated background concentrations. The latter are significantly larger than the local source contributions (as calculated by the model) in Philadelphia and, therefore, play an important role in predicting the GLC of particulate matter. With the PAFS data, we could not readily identify where further improvements can be made to the model; this would require a more extensive and better-defined evaluation data set.

The background concentrations of particulate matter in an urban area are determined by the primary emissions, chemical transformation, and transport on scales much larger than the city size. The background concentrations in Philadelphia are large because of its proximity to other densely-populated urban and industrial centers in the eastern U.S. The relatively smaller contributions from the local sources of particulate matter are determined essentially by the given emissions and meteorology. Therefore, additional effort should be directed towards an examination of the emissions characterization, input meteorology, and variability of background concentrations. An objective methodology to determine the background particulate concentrations should be evolved and the monitoring stations in the field programs in future should be located accordingly.

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